Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:25 PM UTC

PDB ID	:	8K47 / pdb_00008k47
EMDB ID	:	EMD-36879
Title	:	A potent and broad-spectrum neutralizing nanobody for SARS-CoV-2 viruses including all major Omicron strains
Authors	:	Lu, Y.; Gao, Y.; Yao, H.; Xu, W.; Yang, H.
Deposited on	:	2023-07-17
Resolution	:	3.54 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

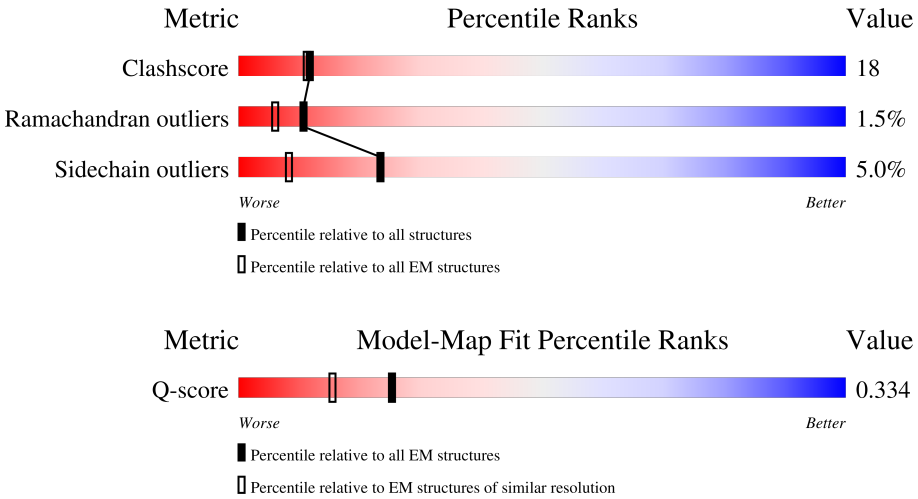
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12891 (3.04 - 4.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	124	44% 59% 41%
2	A	1288	18% 53% 29% • 16%
2	B	1288	15% 53% 27% • 16%
2	C	1288	• 55% 26% • 16%

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Mol	Chain	Length	Quality of chain
3	J	2	100%
3	K	2	50% 50%
3	L	2	100%
3	M	2	100%
3	N	2	100%
3	R	2	50% 50%
3	S	2	100%
3	T	2	100%
3	U	2	100%
3	X	2	100%
3	Y	2	100%
3	Z	2	50% 50%
3	a	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26919 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called nanobody Nb4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	124	Total	C	N	O	S	1	0
			987	623	168	191	5		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1085	Total	C	N	O	S	0	0
			8385	5355	1387	1605	38		
2	B	1084	Total	C	N	O	S	0	0
			8410	5375	1389	1608	38		
2	C	1086	Total	C	N	O	S	0	0
			8437	5400	1391	1608	38		

There are 354 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	conflict	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	658	SER	ASN	conflict	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	19	ILE	THR	conflict	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	658	SER	ASN	conflict	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	conflict	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	658	SER	ASN	conflict	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2

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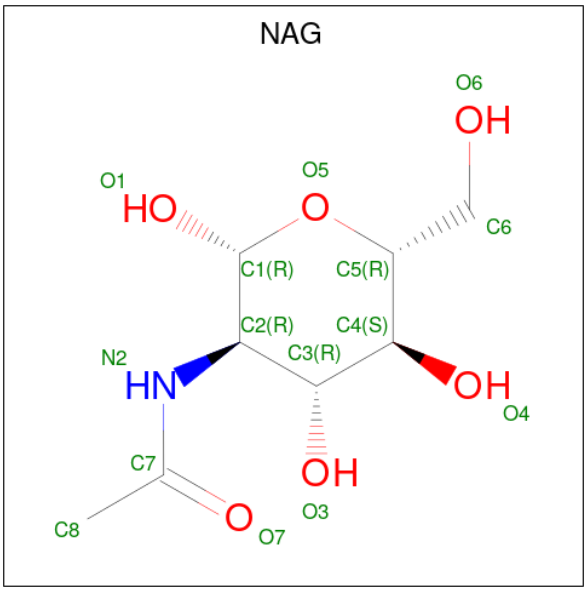
Chain	Residue	Modelled	Actual	Comment	Reference
C	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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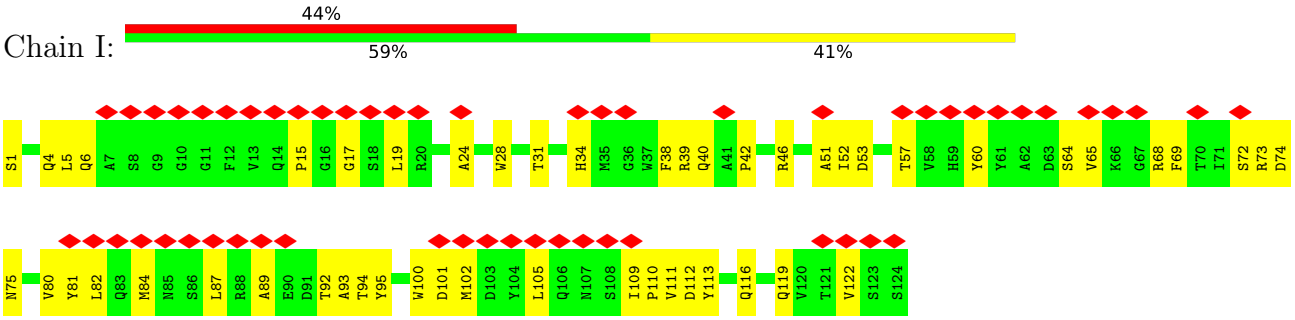
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

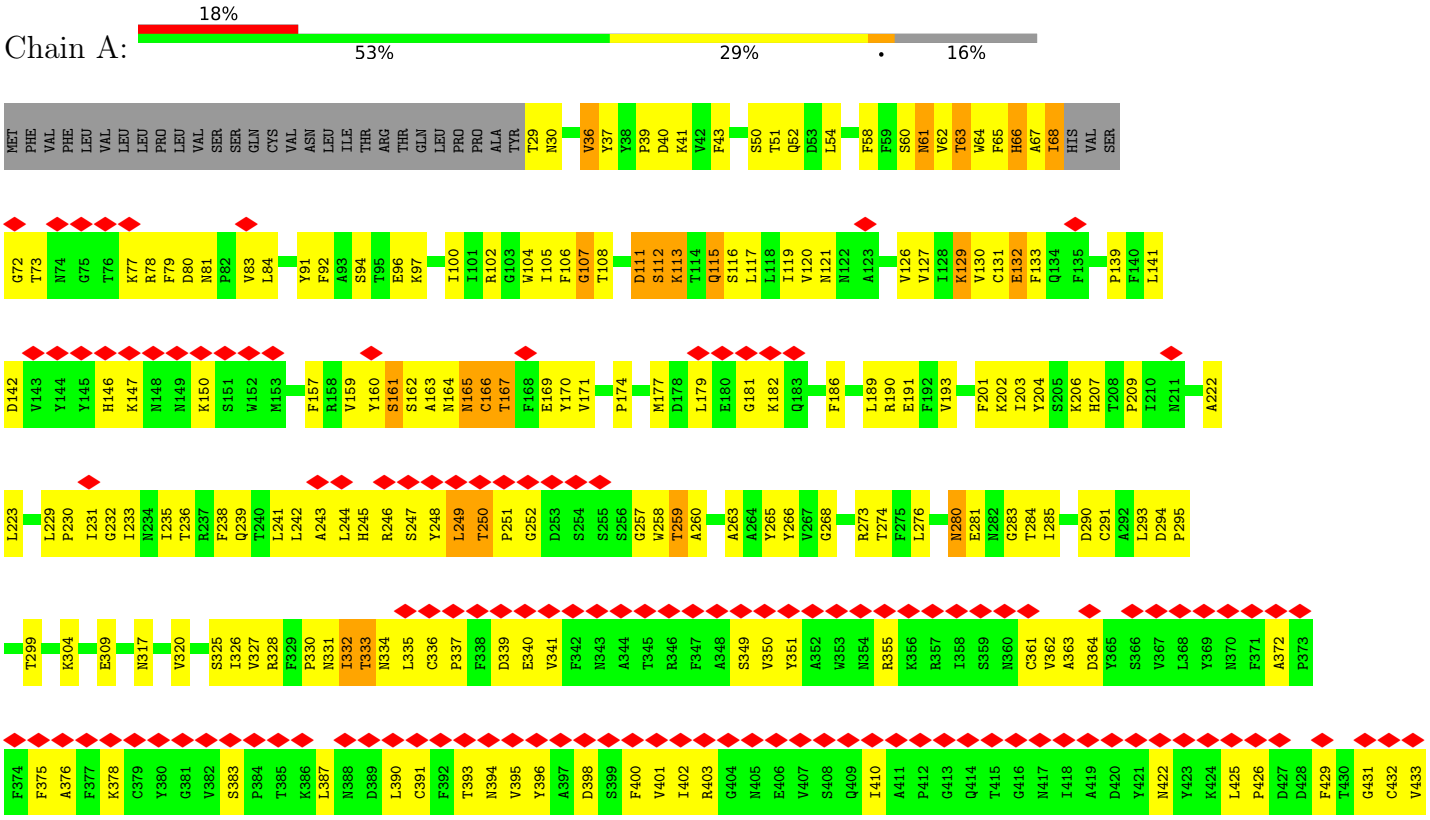
3 Residue-property plots (i)

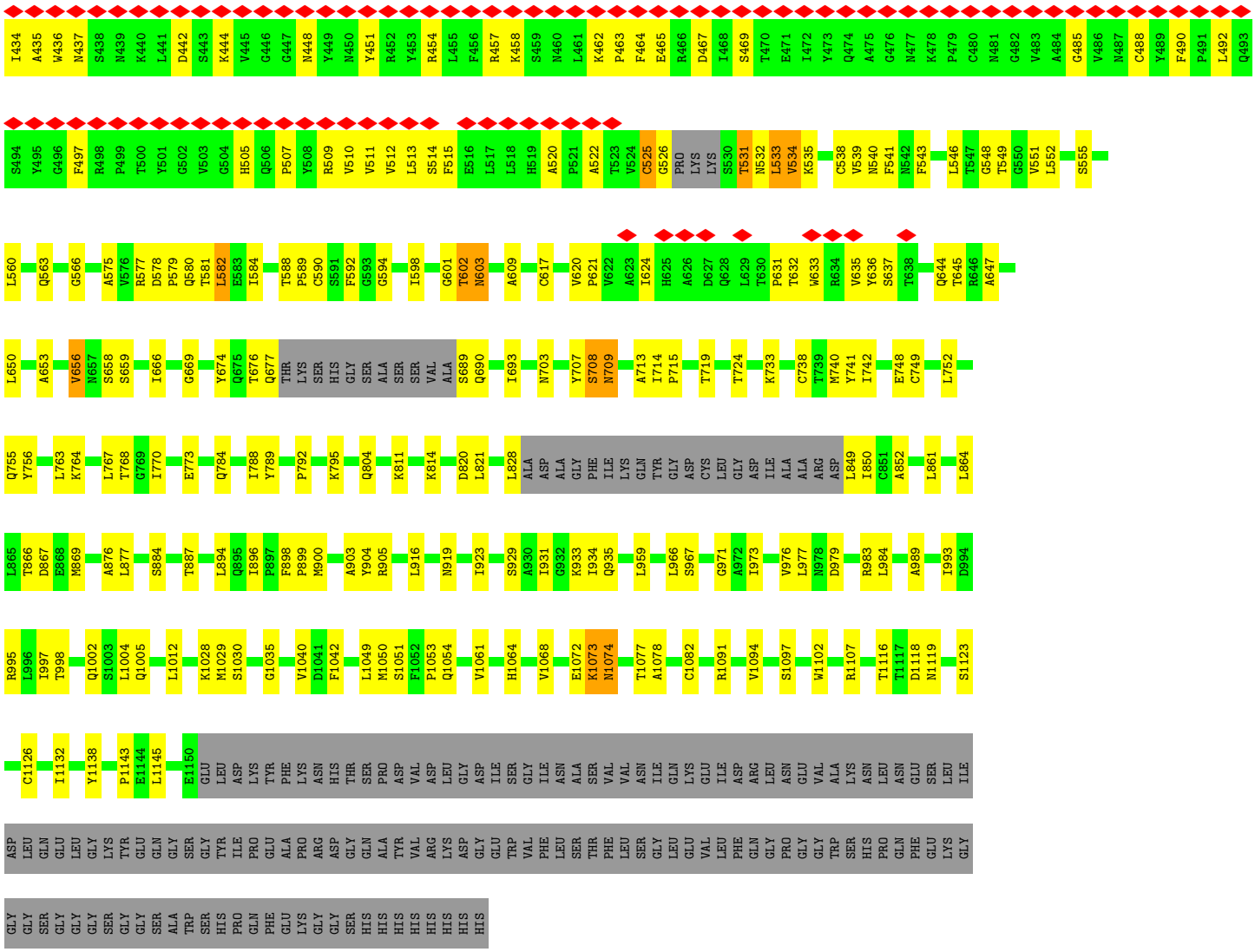
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: nanobody Nb4



• Molecule 2: Spike glycoprotein

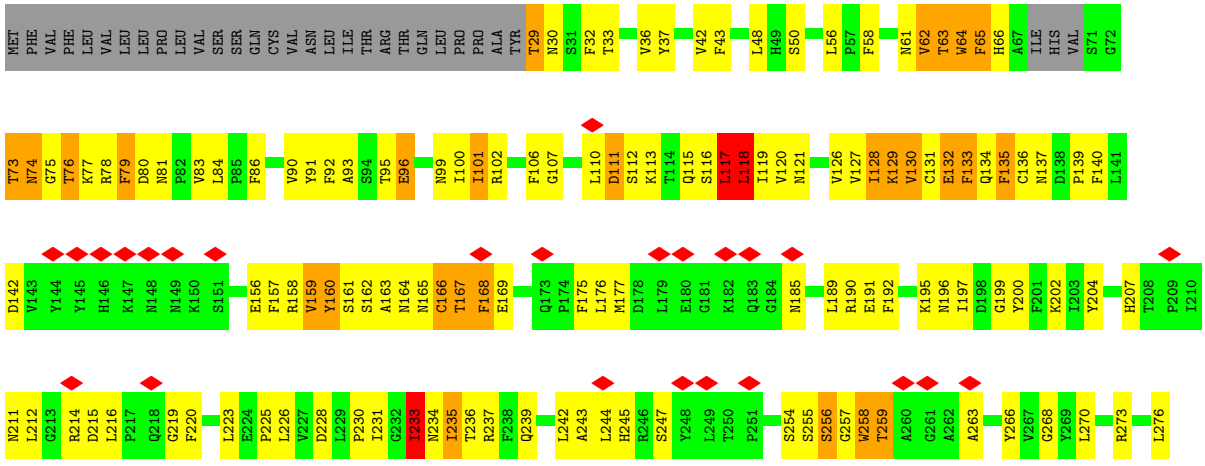


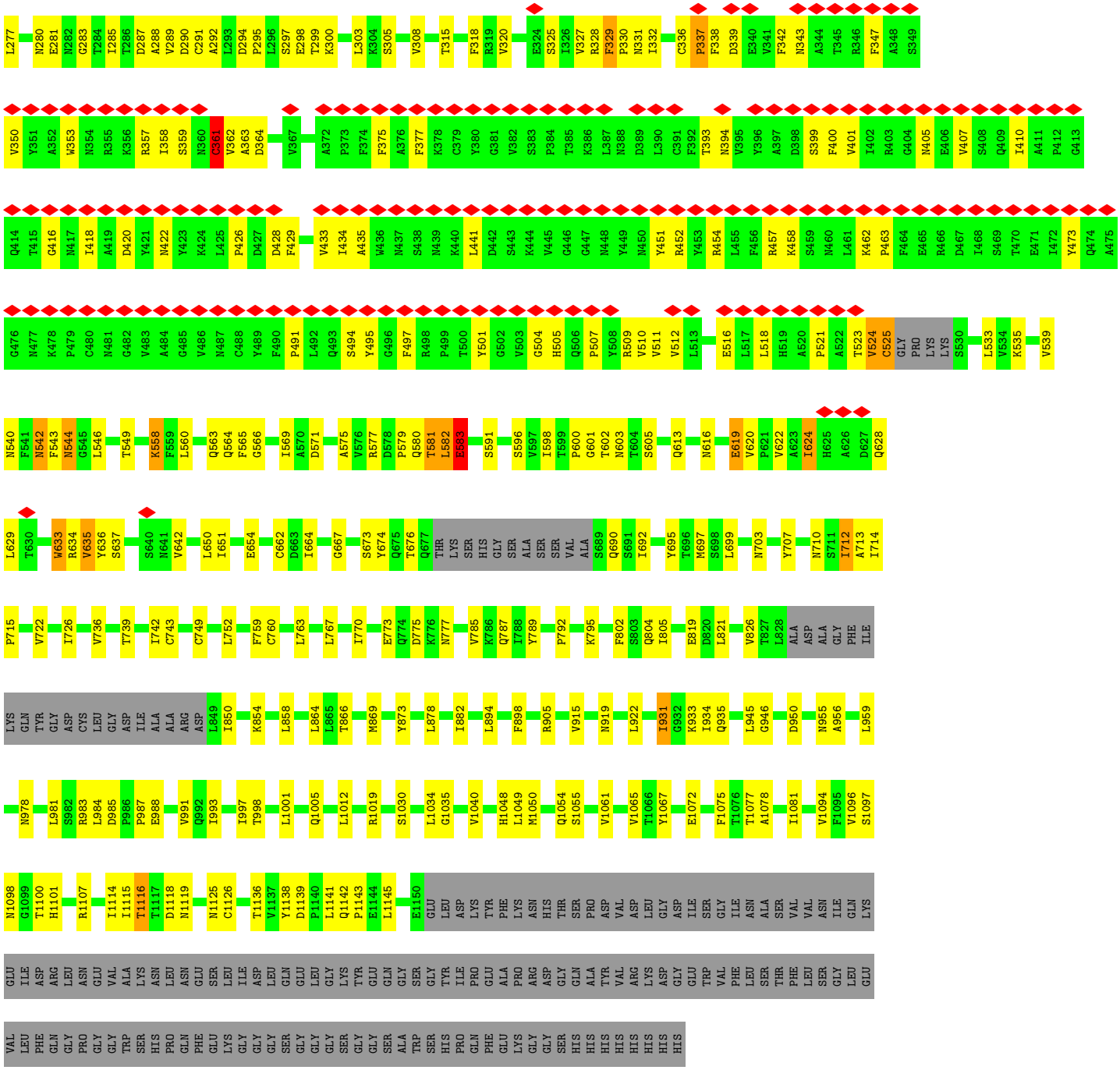


• Molecule 2: Spike glycoprotein

Chain B:



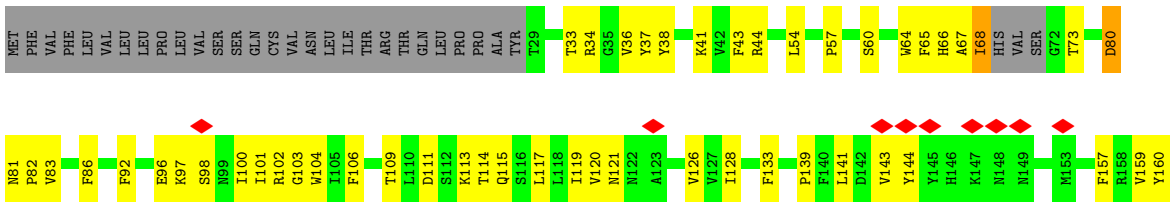


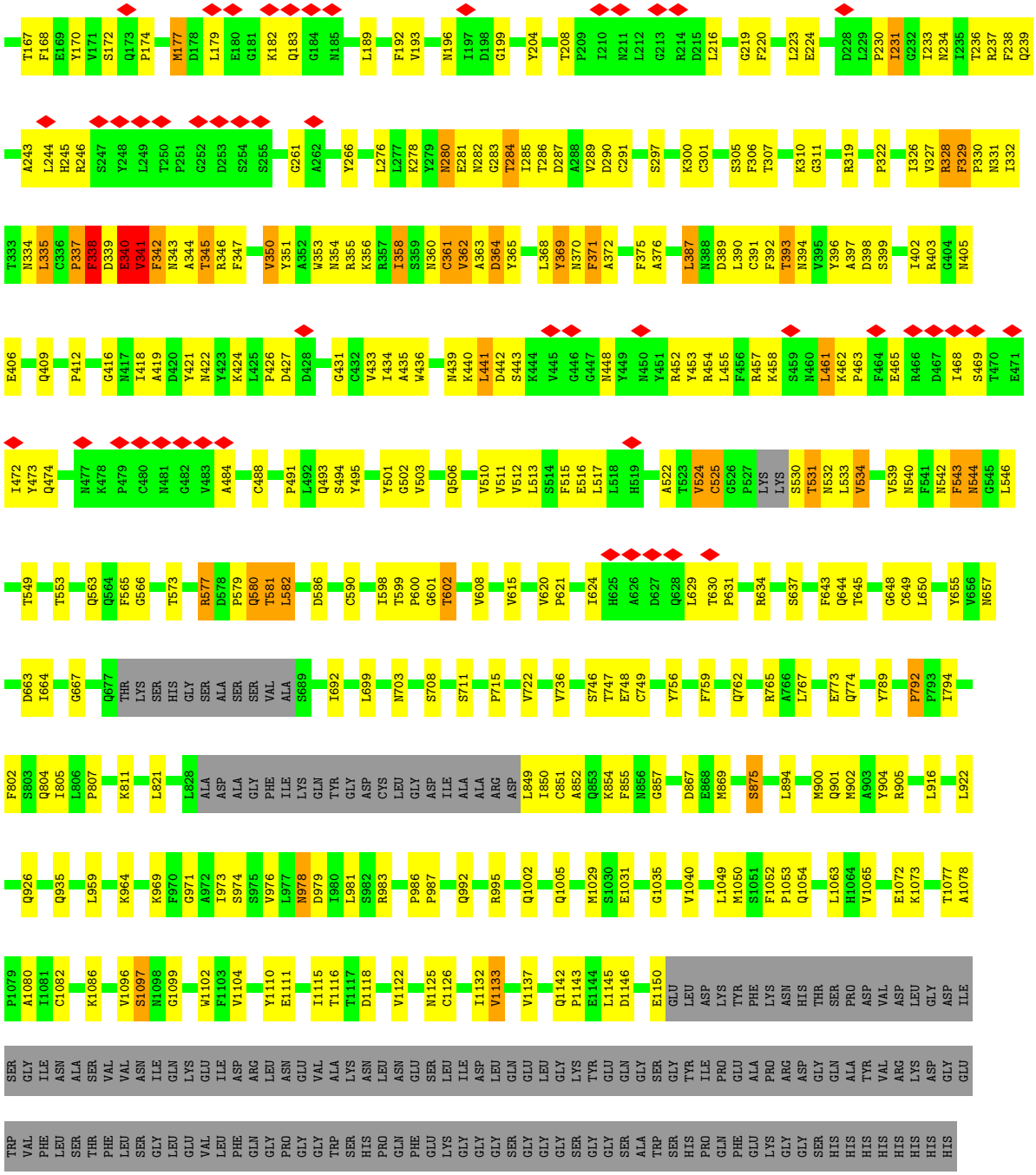


• Molecule 2: Spike glycoprotein

Chain C:

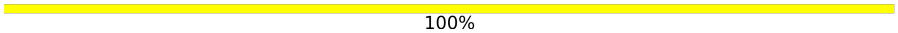






• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

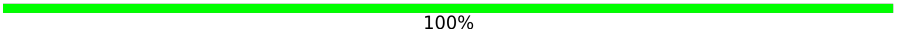
Chain K:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

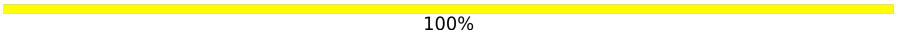
Chain L:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

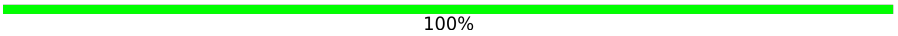
Chain M:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

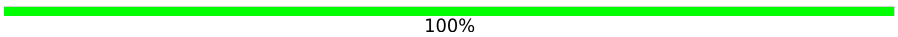
Chain R:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

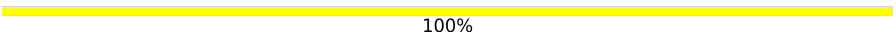
Chain S:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

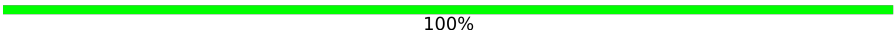
Chain T:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

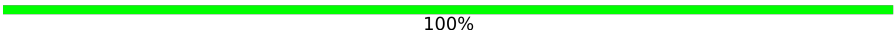
Chain U:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

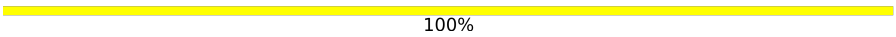
Chain X:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

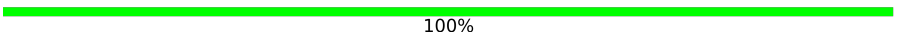
Chain Z:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40530	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.481	Depositor
Minimum map value	-0.504	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	417.792, 417.792, 417.792	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.816, 0.816, 0.816	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	I	0.12	0/1016	0.29	0/1382
2	A	0.36	0/8585	0.55	4/11703 (0.0%)
2	B	0.41	0/8612	0.62	7/11735 (0.1%)
2	C	0.37	0/8642	0.57	2/11776 (0.0%)
All	All	0.37	0/26855	0.57	13/36596 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	361	CYS	CB-CA-C	-9.65	102.34	114.40
2	B	159	VAL	N-CA-C	-7.79	102.13	110.23
2	A	107	GLY	CA-C-O	-6.62	117.68	122.45
2	B	64	TRP	N-CA-C	-6.47	105.49	113.19
2	B	542	ASN	N-CA-C	-5.43	105.36	112.41
2	B	258	TRP	N-CA-C	-5.41	104.46	111.71
2	A	251	PRO	N-CA-C	5.38	119.67	110.74
2	B	168	PHE	CA-C-N	-5.24	113.66	123.03
2	B	168	PHE	C-N-CA	-5.24	113.66	123.03
2	A	251	PRO	CB-CA-C	-5.09	107.59	111.87
2	C	81	ASN	CB-CA-C	5.08	115.52	110.33
2	A	250	THR	CB-CA-C	5.07	117.23	110.13
2	C	792	PRO	O-C-N	-5.03	119.00	121.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	987	0	906	44	0
2	A	8385	0	8083	319	0
2	B	8410	0	8134	317	0
2	C	8437	0	8165	300	0
3	J	28	0	25	0	0
3	K	28	0	25	2	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
4	A	112	0	104	2	0
4	B	112	0	104	1	0
4	C	112	0	104	1	0
All	All	26919	0	25925	930	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (930) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:328:ARG:CB	2:C:328:ARG:HH11	1.58	1.17
2:C:328:ARG:HH11	2:C:328:ARG:HB2	1.07	1.13
2:C:337:PRO:HD3	2:C:364:ASP:HA	1.33	1.07
2:B:134:GLN:HB3	2:B:161:SER:HB2	1.42	1.02
2:B:137:ASN:HB2	2:B:159:VAL:HA	1.49	0.94
2:B:330:PRO:HA	2:B:579:PRO:HB2	1.50	0.91
2:A:29:THR:HA	2:A:260:ALA:HA	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:328:ARG:HB2	2:C:328:ARG:NH1	1.89	0.87
2:B:363:ALA:HB2	2:B:525:CYS:HA	1.57	0.86
2:C:353:TRP:HB2	2:C:398:ASP:HB3	1.54	0.86
2:B:583:GLU:HA	2:B:583:GLU:OE1	1.75	0.84
2:B:295:PRO:HD3	2:B:633:TRP:HD1	1.42	0.84
2:C:393:THR:HA	2:C:522:ALA:HA	1.60	0.83
2:C:335:LEU:HA	2:C:360:ASN:HA	1.59	0.83
2:C:328:ARG:NH2	2:C:543:PHE:CD1	2.46	0.82
2:A:63:THR:HA	2:A:257:GLY:HA2	1.62	0.82
2:A:738:CYS:HB3	2:A:742:ILE:HD12	1.60	0.82
2:C:167:THR:HG22	2:C:168:PHE:H	1.44	0.81
2:A:327:VAL:HG23	2:A:531:THR:HA	1.63	0.80
2:C:328:ARG:NH1	2:C:328:ARG:H	1.79	0.79
2:C:337:PRO:C	2:C:339:ASP:H	1.91	0.79
2:C:328:ARG:CB	2:C:328:ARG:NH1	2.42	0.78
2:A:120:VAL:HB	2:A:127:VAL:HB	1.65	0.78
1:I:73:ARG:HA	1:I:80:VAL:HA	1.67	0.77
2:C:350:VAL:HB	2:C:402:ILE:HG22	1.65	0.77
2:A:645:THR:HG22	2:A:647:ALA:H	1.50	0.76
2:C:350:VAL:HG21	2:C:418:ILE:HG12	1.67	0.76
2:B:63:THR:HB	2:B:65:PHE:HD1	1.50	0.76
2:B:83:VAL:HG21	2:B:237:ARG:HE	1.51	0.76
1:I:92:THR:HG22	1:I:122:VAL:H	1.51	0.75
2:C:364:ASP:HB2	2:C:524:VAL:HG12	1.67	0.75
2:A:575:ALA:HB1	2:A:584:ILE:HD11	1.68	0.75
2:C:375:PHE:HB3	2:C:436:TRP:HB3	1.69	0.75
2:A:770:ILE:HD11	2:A:1012:LEU:HD23	1.69	0.74
2:A:1094:VAL:HG23	2:C:900:MET:HE1	1.70	0.74
2:B:106:PHE:HB3	2:B:235:ILE:HD12	1.70	0.73
2:C:280:ASN:HD21	2:C:284:THR:HG23	1.53	0.73
2:B:139:PRO:HB3	2:B:243:ALA:HB2	1.71	0.73
2:C:204:TYR:HB3	2:C:223:LEU:HB3	1.70	0.72
2:C:356:LYS:HB2	2:C:397:ALA:HB3	1.71	0.72
2:C:553:THR:HG23	2:C:586:ASP:HB3	1.72	0.72
2:B:64:TRP:H	2:B:259:THR:HG23	1.54	0.72
2:B:560:LEU:HD13	2:B:563:GLN:HG3	1.73	0.71
2:A:65:PHE:CD1	2:A:67:ALA:HB2	2.26	0.71
2:C:644:GLN:HA	2:C:649:CYS:HB2	1.72	0.71
2:C:354:ASN:H	2:C:399:SER:H	1.38	0.71
2:A:904:TYR:CE2	2:B:1107:ARG:HG2	2.27	0.70
2:C:83:VAL:HG23	2:C:239:GLN:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:THR:HG21	2:B:518:LEU:HB2	1.73	0.69
2:B:422:ASN:ND2	2:B:454:ARG:O	2.24	0.69
2:B:295:PRO:HD3	2:B:633:TRP:CD1	2.26	0.69
2:C:372:ALA:HB3	2:C:375:PHE:HD2	1.57	0.69
2:B:107:GLY:H	2:B:235:ILE:HG23	1.57	0.69
2:C:83:VAL:HG21	2:C:237:ARG:HH21	1.56	0.68
2:C:973:ILE:HD12	2:C:973:ILE:H	1.57	0.68
2:C:452:ARG:HG2	2:C:494:SER:HA	1.76	0.68
2:C:1053:PRO:O	2:C:1054:GLN:NE2	2.27	0.68
2:A:30:ASN:HA	2:A:61:ASN:HB2	1.76	0.67
2:B:338:PHE:HE2	2:B:364:ASP:HB3	1.59	0.67
1:I:100:TRP:HD1	1:I:111:VAL:HG22	1.58	0.67
2:B:984:LEU:HD23	2:B:988:GLU:HG3	1.74	0.67
2:B:850:ILE:O	2:B:854:LYS:NZ	2.26	0.67
2:A:330:PRO:HG3	2:A:531:THR:HG21	1.77	0.67
2:A:971:GLY:O	2:A:995:ARG:NH1	2.27	0.67
2:A:102:ARG:NH2	2:A:121:ASN:O	2.28	0.66
2:B:405:ASN:N	2:B:504:GLY:O	2.28	0.66
2:C:1086:LYS:HD2	2:C:1122:VAL:HG11	1.77	0.66
2:A:133:PHE:HA	2:A:162:SER:HA	1.77	0.66
2:A:1053:PRO:O	2:A:1054:GLN:NE2	2.27	0.66
2:A:193:VAL:HB	2:A:204:TYR:HB2	1.77	0.66
2:B:185:ASN:HA	2:B:211:ASN:HB2	1.78	0.66
2:B:137:ASN:CB	2:B:159:VAL:HA	2.23	0.66
1:I:109:ILE:HG23	1:I:110:PRO:HD3	1.77	0.66
2:C:245:HIS:O	2:C:245:HIS:ND1	2.29	0.66
2:B:451:TYR:HB3	2:B:495:TYR:HD2	1.62	0.65
2:C:773:GLU:OE1	2:C:774:GLN:NE2	2.29	0.65
2:B:407:VAL:HA	2:B:410:ILE:HD12	1.77	0.65
2:B:915:VAL:O	2:B:919:ASN:ND2	2.30	0.65
2:C:804:GLN:NE2	2:C:935:GLN:OE1	2.25	0.65
1:I:64:SER:O	1:I:68:ARG:NH2	2.30	0.65
2:C:372:ALA:H	2:C:375:PHE:HE2	1.44	0.65
2:C:922:LEU:HD11	3:K:1:NAG:H5	1.79	0.65
2:A:206:LYS:NZ	2:A:207:HIS:O	2.29	0.64
2:B:873:TYR:HE1	2:C:699:LEU:HB3	1.61	0.64
2:B:434:ILE:HB	2:B:511:VAL:HB	1.78	0.64
2:C:328:ARG:NH1	2:C:328:ARG:N	2.44	0.64
2:B:418:ILE:HD12	2:B:422:ASN:HD22	1.62	0.64
2:A:117:LEU:HD13	2:A:235:ILE:HD11	1.80	0.64
2:A:540:ASN:HA	2:A:549:THR:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:TYR:HD1	2:C:502:GLY:H	1.46	0.64
2:A:147:LYS:HA	2:A:246:ARG:HA	1.79	0.64
2:B:426:PRO:HB3	2:B:463:PRO:HB3	1.79	0.64
2:B:133:PHE:HA	2:B:162:SER:HA	1.80	0.64
2:B:1005:GLN:OE1	2:C:1002:GLN:NE2	2.30	0.64
2:A:117:LEU:HG	2:A:130:VAL:HG13	1.80	0.63
2:B:102:ARG:HH12	2:B:156:GLU:HG3	1.61	0.63
2:A:620:VAL:HG22	2:A:621:PRO:HD3	1.79	0.63
2:B:338:PHE:HD1	2:B:342:PHE:HE2	1.47	0.63
2:C:422:ASN:ND2	2:C:454:ARG:O	2.30	0.63
2:A:811:LYS:O	2:A:814:LYS:NZ	2.31	0.63
2:C:361:CYS:SG	2:C:362:VAL:N	2.65	0.63
2:A:804:GLN:NE2	2:A:935:GLN:OE1	2.30	0.63
2:B:130:VAL:HB	2:B:167:THR:HG23	1.79	0.63
2:B:303:LEU:HD22	2:B:308:VAL:HG12	1.80	0.63
2:B:320:VAL:HG13	2:B:628:GLN:HE22	1.62	0.63
2:C:34:ARG:NH1	2:C:219:GLY:O	2.32	0.63
2:A:115:GLN:HB3	2:A:130:VAL:HG12	1.79	0.63
2:B:133:PHE:O	2:B:134:GLN:C	2.42	0.63
2:C:103:GLY:HA3	2:C:120:VAL:HA	1.79	0.63
2:C:852:ALA:HA	2:C:855:PHE:CZ	2.33	0.63
1:I:28:TRP:HE1	2:C:369:TYR:HB3	1.64	0.63
2:A:904:TYR:HE2	2:B:1107:ARG:HG2	1.64	0.62
2:C:328:ARG:HH11	2:C:328:ARG:CA	2.11	0.62
2:C:337:PRO:C	2:C:339:ASP:N	2.57	0.62
1:I:100:TRP:CD1	1:I:111:VAL:HG22	2.33	0.62
2:A:40:ASP:OD1	2:A:41:LYS:N	2.28	0.62
2:A:444:LYS:HE2	2:A:448:ASN:HA	1.81	0.62
2:A:601:GLY:O	2:A:602:THR:C	2.41	0.62
2:B:111:ASP:HA	2:B:135:PHE:HA	1.80	0.62
2:C:328:ARG:NH2	2:C:543:PHE:CE1	2.67	0.62
2:A:65:PHE:HD1	2:A:67:ALA:HB2	1.65	0.62
2:A:635:VAL:HG13	2:A:636:TYR:HD1	1.65	0.62
2:C:67:ALA:O	2:C:68:ILE:C	2.42	0.62
2:C:600:PRO:HD3	2:C:692:ILE:HD11	1.81	0.62
2:B:64:TRP:HB3	2:B:263:ALA:HB3	1.82	0.62
2:B:214:ARG:NH1	2:B:216:LEU:O	2.32	0.62
2:B:127:VAL:HG13	2:B:169:GLU:HG3	1.82	0.62
2:C:394:ASN:HB3	2:C:516:GLU:HB3	1.82	0.62
2:A:393:THR:OG1	2:A:394:ASN:OD1	2.18	0.62
2:B:102:ARG:HD3	2:B:244:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:ASN:HB3	2:B:579:PRO:HB3	1.82	0.62
2:C:372:ALA:HB3	2:C:375:PHE:CD2	2.35	0.62
2:C:387:LEU:HD12	2:C:392:PHE:HZ	1.65	0.61
2:C:409:GLN:HB3	2:C:419:ALA:HB2	1.83	0.61
2:B:581:THR:O	2:B:583:GLU:N	2.33	0.61
2:C:337:PRO:O	2:C:339:ASP:N	2.31	0.61
2:C:746:SER:HB2	2:C:749:CYS:HB3	1.82	0.61
2:A:293:LEU:HD23	2:A:294:ASP:HB2	1.83	0.61
2:B:983:ARG:HG2	2:C:390:LEU:HD21	1.83	0.61
2:C:491:PRO:O	2:C:493:GLN:NE2	2.34	0.61
2:C:624:ILE:HG21	2:C:629:LEU:HD13	1.83	0.61
2:C:353:TRP:CB	2:C:398:ASP:HB3	2.30	0.61
2:C:68:ILE:HB	2:C:80:ASP:HA	1.83	0.60
2:C:139:PRO:HA	2:C:157:PHE:HA	1.83	0.60
2:A:1002:GLN:NE2	2:C:1005:GLN:OE1	2.34	0.60
2:B:96:GLU:HG3	2:B:101:ILE:H	1.66	0.60
2:B:102:ARG:NH1	2:B:243:ALA:O	2.34	0.60
2:A:560:LEU:O	2:A:577:ARG:NH2	2.35	0.60
2:A:602:THR:O	2:A:603:ASN:C	2.45	0.60
2:A:811:LYS:NZ	2:A:820:ASP:OD2	2.26	0.60
2:B:569:ILE:HG13	2:B:569:ILE:O	2.01	0.60
2:C:620:VAL:HB	2:C:621:PRO:HD3	1.83	0.60
2:A:117:LEU:CD1	2:A:235:ILE:HD11	2.32	0.60
2:A:355:ARG:HH12	2:A:464:PHE:HB3	1.67	0.59
2:A:91:TYR:N	2:A:268:GLY:O	2.26	0.59
2:C:341:VAL:O	2:C:342:PHE:C	2.45	0.59
2:A:429:PHE:HE1	2:A:514:SER:HB3	1.67	0.59
2:B:83:VAL:HG23	2:B:239:GLN:HG2	1.84	0.59
2:A:177:MET:HE2	2:A:179:LEU:HD21	1.83	0.59
2:B:566:GLY:HA3	2:B:575:ALA:HB3	1.83	0.59
2:B:117:LEU:HG	2:B:130:VAL:HG13	1.85	0.59
2:B:451:TYR:HB3	2:B:495:TYR:CD2	2.37	0.59
2:B:1138:TYR:HE1	2:B:1143:PRO:HG2	1.67	0.59
2:C:102:ARG:HB2	2:C:243:ALA:HB3	1.83	0.59
2:C:362:VAL:HG22	2:C:363:ALA:H	1.67	0.59
2:A:142:ASP:HB2	2:A:146:HIS:HB3	1.83	0.59
2:A:396:TYR:N	2:A:514:SER:O	2.32	0.59
2:A:1116:THR:OG1	2:A:1118:ASP:OD1	2.21	0.58
2:B:80:ASP:O	2:B:81:ASN:C	2.46	0.58
1:I:1:SER:O	1:I:113:TYR:OH	2.20	0.58
2:B:64:TRP:O	2:B:65:PHE:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:VAL:HB	2:B:167:THR:CG2	2.32	0.58
2:B:159:VAL:O	2:B:160:TYR:C	2.46	0.58
2:C:1031:GLU:N	2:C:1031:GLU:OE2	2.36	0.58
2:A:738:CYS:O	2:A:742:ILE:N	2.33	0.58
2:C:356:LYS:HB3	2:C:358:ILE:HG23	1.84	0.58
2:A:263:ALA:N	2:A:266:TYR:OH	2.36	0.58
2:B:426:PRO:HG2	2:B:429:PHE:HB2	1.85	0.58
2:A:866:THR:HG22	2:A:869:MET:HE3	1.86	0.58
2:A:1126:CYS:HB2	2:A:1132:ILE:HD13	1.85	0.58
2:A:117:LEU:HD21	2:A:233:ILE:HD13	1.85	0.58
2:C:354:ASN:HD21	2:C:356:LYS:HG2	1.69	0.58
2:B:129:LYS:HE3	2:B:168:PHE:HA	1.84	0.58
2:B:600:PRO:HD3	2:B:692:ILE:HD11	1.85	0.58
2:C:34:ARG:HG3	2:C:216:LEU:HD23	1.85	0.58
2:A:320:VAL:HG13	2:A:590:CYS:HB2	1.85	0.58
2:A:328:ARG:HH21	2:A:533:LEU:HA	1.69	0.58
2:B:673:SER:HB3	2:B:695:TYR:HE2	1.69	0.57
2:C:439:ASN:O	2:C:443:SER:OG	2.20	0.57
2:A:398:ASP:O	2:A:512:VAL:N	2.35	0.57
2:A:433:VAL:HG22	2:A:512:VAL:HG22	1.86	0.57
2:A:555:SER:HB3	2:A:584:ILE:HG23	1.86	0.57
2:C:503:VAL:HA	2:C:506:GLN:HB2	1.85	0.57
2:C:722:VAL:HG22	2:C:1065:VAL:HG22	1.86	0.57
2:B:434:ILE:N	2:B:511:VAL:O	2.37	0.57
2:C:849:LEU:HG	2:C:851:CYS:H	1.69	0.57
2:A:749:CYS:SG	2:A:997:ILE:HD11	2.44	0.57
2:C:337:PRO:CD	2:C:364:ASP:HA	2.22	0.57
2:A:674:TYR:CZ	2:A:690:GLN:HB3	2.39	0.57
2:B:353:TRP:HB3	2:B:400:PHE:HD2	1.69	0.57
2:C:426:PRO:HD3	2:C:463:PRO:HB3	1.87	0.57
2:A:401:VAL:HG22	2:A:509:ARG:HG2	1.87	0.56
2:C:976:VAL:HG12	2:C:979:ASP:H	1.69	0.56
2:C:1142:GLN:OE1	2:C:1143:PRO:HD3	2.05	0.56
2:A:331:ASN:O	2:A:580:GLN:HA	2.05	0.56
2:C:926:GLN:NE2	3:K:1:NAG:O6	2.38	0.56
1:I:4:GLN:N	1:I:4:GLN:OE1	2.39	0.56
2:B:327:VAL:HG23	2:B:533:LEU:HA	1.88	0.56
2:B:328:ARG:C	2:B:330:PRO:HD3	2.30	0.56
2:B:336:CYS:HB3	2:B:338:PHE:CZ	2.41	0.56
2:C:339:ASP:O	2:C:341:VAL:HG12	2.05	0.56
2:A:391:CYS:HB3	2:A:522:ALA:HB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:LYS:HG3	2:B:473:TYR:HD1	1.71	0.56
2:B:821:LEU:HD22	2:B:935:GLN:HG3	1.87	0.56
2:C:387:LEU:HD12	2:C:392:PHE:CZ	2.40	0.56
2:A:317:ASN:HA	2:A:594:GLY:HA2	1.87	0.56
2:B:290:ASP:OD1	2:B:292:ALA:N	2.33	0.56
2:B:736:VAL:HG23	2:B:858:LEU:HD23	1.87	0.56
2:C:44:ARG:O	2:C:283:GLY:HA2	2.05	0.56
2:B:73:THR:O	2:B:74:ASN:C	2.49	0.56
2:B:636:TYR:O	2:B:637:SER:C	2.49	0.56
2:A:676:THR:OG1	2:A:689:SER:OG	2.23	0.56
2:B:81:ASN:HD21	2:B:242:LEU:HG	1.70	0.56
2:B:190:ARG:HB3	2:B:192:PHE:CE2	2.40	0.56
2:C:540:ASN:OD1	2:C:549:THR:OG1	2.21	0.56
2:A:395:VAL:HG22	2:A:515:PHE:HB3	1.88	0.56
2:A:139:PRO:HG3	2:A:243:ALA:HA	1.87	0.56
2:C:339:ASP:O	2:C:341:VAL:N	2.38	0.56
2:A:83:VAL:HA	2:A:239:GLN:HG2	1.87	0.55
2:A:202:LYS:NZ	2:A:203:ILE:O	2.39	0.55
2:A:589:PRO:HG3	2:C:855:PHE:CD1	2.41	0.55
2:C:867:ASP:N	2:C:867:ASP:OD1	2.39	0.55
2:A:437:ASN:ND2	2:A:507:PRO:O	2.38	0.55
2:B:583:GLU:OE1	2:B:583:GLU:CA	2.51	0.55
2:C:355:ARG:HA	2:C:396:TYR:HE1	1.70	0.55
2:A:77:LYS:HG2	2:A:79:PHE:H	1.72	0.55
2:B:955:ASN:OD1	2:B:956:ALA:N	2.39	0.55
2:B:353:TRP:HB2	2:B:399:SER:H	1.71	0.55
2:B:582:LEU:O	2:B:583:GLU:C	2.49	0.55
1:I:6:GLN:HB2	1:I:24:ALA:HB3	1.87	0.55
2:B:560:LEU:HD12	2:B:560:LEU:H	1.72	0.55
2:B:273:ARG:NH1	2:B:290:ASP:OD2	2.40	0.55
2:B:676:THR:N	2:B:690:GLN:OE1	2.40	0.55
2:C:337:PRO:HA	2:C:358:ILE:HB	1.87	0.55
2:A:541:PHE:N	2:A:548:GLY:O	2.36	0.55
2:B:91:TYR:HB3	2:B:268:GLY:HA3	1.89	0.55
2:B:280:ASN:OD1	2:B:281:GLU:N	2.39	0.55
2:B:714:ILE:HD12	2:B:1096:VAL:HG11	1.88	0.55
2:C:979:ASP:O	2:C:983:ARG:HB2	2.06	0.55
2:A:1077:THR:OG1	2:A:1078:ALA:N	2.38	0.55
2:B:212:LEU:HD12	2:B:215:ASP:HA	1.87	0.55
2:C:756:TYR:HB3	2:C:759:PHE:HD2	1.71	0.55
2:A:131:CYS:HA	2:A:166:CYS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:580:GLN:O	2:C:582:LEU:N	2.41	0.54
2:B:1005:GLN:CD	2:C:1002:GLN:HE22	2.15	0.54
2:A:41:LYS:HG2	2:B:564:GLN:HG2	1.88	0.54
2:A:355:ARG:NH2	2:A:398:ASP:OD2	2.40	0.54
2:A:372:ALA:H	2:A:375:PHE:HE2	1.54	0.54
2:A:1040:VAL:HG21	2:C:1035:GLY:HA3	1.88	0.54
2:B:338:PHE:HD1	2:B:342:PHE:CE2	2.26	0.54
2:C:189:LEU:HB2	2:C:208:THR:HB	1.90	0.54
2:B:117:LEU:HD22	2:B:119:ILE:HD11	1.88	0.54
2:B:287:ASP:OD1	2:B:288:ALA:N	2.41	0.54
2:C:1116:THR:OG1	2:C:1118:ASP:OD1	2.24	0.54
2:A:713:ALA:HB3	2:C:894:LEU:HB3	1.90	0.54
2:C:902:MET:HB3	2:C:916:LEU:HD11	1.89	0.54
1:I:42:PRO:HD3	1:I:93:ALA:HB2	1.90	0.54
2:A:165:ASN:O	2:A:166:CYS:C	2.51	0.54
2:B:115:GLN:HB2	2:B:233:ILE:HG13	1.89	0.54
2:B:350:VAL:HA	2:B:400:PHE:HB2	1.88	0.54
2:C:290:ASP:OD1	2:C:291:CYS:N	2.40	0.54
2:B:119:ILE:HG12	2:B:128:ILE:HG23	1.90	0.54
2:B:290:ASP:OD1	2:B:291:CYS:N	2.41	0.54
2:C:563:GLN:O	2:C:577:ARG:NH1	2.41	0.54
2:C:621:PRO:HA	2:C:624:ILE:HG23	1.90	0.54
1:I:40:GLN:HB3	1:I:46:ARG:HD3	1.89	0.54
2:A:378:LYS:HG3	2:A:433:VAL:HB	1.89	0.54
2:A:621:PRO:HA	2:A:624:ILE:HG23	1.89	0.54
2:C:762:GLN:HE22	2:C:765:ARG:HH12	1.56	0.54
2:B:792:PRO:O	2:B:795:LYS:NZ	2.41	0.53
2:B:295:PRO:O	2:B:299:THR:HG23	2.07	0.53
1:I:40:GLN:HB3	1:I:46:ARG:HA	1.89	0.53
2:A:497:PHE:CZ	2:A:507:PRO:HB3	2.44	0.53
2:B:726:ILE:HD12	2:B:1061:VAL:HG22	1.90	0.53
2:B:64:TRP:CE3	2:B:263:ALA:HB3	2.43	0.53
2:B:773:GLU:HG3	2:B:1019:ARG:NH2	2.23	0.53
2:A:30:ASN:HA	2:A:61:ASN:HA	1.90	0.53
2:A:177:MET:O	2:A:190:ARG:NH2	2.34	0.53
2:C:326:ILE:HG12	2:C:539:VAL:HG11	1.89	0.53
2:C:542:ASN:O	2:C:543:PHE:C	2.51	0.53
2:A:190:ARG:HE	2:A:207:HIS:HB2	1.73	0.53
2:B:256:SER:HA	2:B:259:THR:HG22	1.90	0.53
2:B:454:ARG:HD3	2:B:457:ARG:HG3	1.89	0.53
2:A:617:CYS:HA	2:A:621:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1119:ASN:ND2	2:A:1119:ASN:O	2.42	0.53
2:A:132:GLU:CD	2:A:164:ASN:HB2	2.34	0.53
2:C:340:GLU:O	2:C:341:VAL:C	2.50	0.53
2:C:971:GLY:O	2:C:995:ARG:NH1	2.41	0.53
1:I:73:ARG:HH21	2:C:503:VAL:HG11	1.73	0.53
2:B:501:TYR:HB3	2:B:505:HIS:HB2	1.91	0.53
2:C:978:ASN:HA	2:C:981:LEU:HG	1.91	0.53
2:B:777:ASN:HD21	2:B:1019:ARG:HA	1.73	0.53
2:B:1049:LEU:HD11	2:B:1067:TYR:HB2	1.91	0.53
2:C:98:SER:O	2:C:102:ARG:NH2	2.42	0.53
2:A:578:ASP:OD1	2:A:581:THR:N	2.37	0.52
2:A:620:VAL:CG2	2:A:621:PRO:HD3	2.39	0.52
2:C:109:THR:OG1	2:C:111:ASP:OD1	2.27	0.52
2:C:328:ARG:NH1	2:C:328:ARG:CA	2.71	0.52
2:C:338:PHE:O	2:C:339:ASP:C	2.52	0.52
2:A:29:THR:O	2:A:61:ASN:HA	2.09	0.52
2:B:33:THR:OG1	2:B:219:GLY:O	2.26	0.52
2:B:63:THR:HB	2:B:65:PHE:CD1	2.40	0.52
2:B:133:PHE:HA	2:B:162:SER:CA	2.39	0.52
2:B:1142:GLN:HB3	2:B:1143:PRO:HD3	1.90	0.52
2:C:128:ILE:HG12	2:C:170:TYR:HB3	1.91	0.52
2:A:331:ASN:O	2:A:333:THR:N	2.41	0.52
2:A:431:GLY:HA3	2:A:514:SER:HA	1.91	0.52
2:C:344:ALA:HB3	2:C:347:PHE:HE1	1.72	0.52
2:B:985:ASP:HB2	2:B:987:PRO:HD2	1.91	0.52
2:B:1141:LEU:HG	2:B:1145:LEU:HD23	1.90	0.52
2:A:102:ARG:HG3	2:A:243:ALA:HB3	1.91	0.52
2:A:206:LYS:HB3	2:A:223:LEU:HD23	1.90	0.52
2:A:1091:ARG:NH2	2:A:1118:ASP:O	2.42	0.52
2:A:1097:SER:HB3	2:A:1102:TRP:CE3	2.44	0.52
2:A:29:THR:CA	2:A:260:ALA:HA	2.32	0.52
2:A:485:GLY:H	2:A:488:CYS:HB2	1.74	0.52
2:A:644:GLN:NE2	2:A:645:THR:O	2.43	0.52
2:B:662:CYS:HB2	2:B:697:MET:SD	2.49	0.52
2:B:290:ASP:CG	2:B:292:ALA:H	2.18	0.52
2:B:516:GLU:HB3	2:B:518:LEU:HG	1.92	0.52
2:C:96:GLU:HG2	2:C:101:ILE:HB	1.92	0.52
2:B:298:GLU:HG2	2:B:315:THR:HB	1.92	0.52
2:C:454:ARG:HD2	2:C:457:ARG:HH21	1.75	0.52
2:C:598:ILE:HG23	2:C:664:ILE:HG21	1.92	0.52
2:B:633:TRP:C	2:B:635:VAL:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:739:THR:O	2:B:743:CYS:N	2.35	0.52
2:A:50:SER:HA	2:A:276:LEU:HA	1.92	0.51
2:A:104:TRP:HE3	2:A:119:ILE:HB	1.75	0.51
2:A:538:CYS:HB3	2:A:551:VAL:HG22	1.93	0.51
2:A:784:GLN:OE1	2:A:1030:SER:OG	2.26	0.51
2:B:131:CYS:SG	2:B:167:THR:HG22	2.50	0.51
2:B:159:VAL:O	2:B:161:SER:N	2.43	0.51
2:B:715:PRO:HA	2:B:1072:GLU:HA	1.92	0.51
1:I:19:LEU:H	1:I:84:MET:HG3	1.76	0.51
1:I:28:TRP:HB3	2:C:375:PHE:CE1	2.45	0.51
2:A:295:PRO:O	2:A:299:THR:HG23	2.10	0.51
2:C:278:LYS:HG2	2:C:287:ASP:H	1.75	0.51
2:A:748:GLU:O	2:A:752:LEU:HG	2.10	0.51
2:A:867:ASP:OD1	2:A:867:ASP:N	2.42	0.51
2:A:977:LEU:HD22	2:A:993:ILE:HD12	1.92	0.51
2:A:37:TYR:OH	2:A:54:LEU:O	2.28	0.51
2:A:111:ASP:O	2:A:113:LYS:N	2.44	0.51
2:A:248:TYR:O	2:A:249:LEU:C	2.54	0.51
2:A:330:PRO:O	2:A:579:PRO:HB2	2.10	0.51
2:A:752:LEU:O	2:A:755:GLN:NE2	2.44	0.51
2:A:773:GLU:OE2	2:A:773:GLU:HA	2.10	0.51
2:B:338:PHE:CE2	2:B:364:ASP:HB3	2.43	0.51
2:C:305:SER:OG	2:C:307:THR:O	2.27	0.51
2:B:258:TRP:O	2:B:259:THR:C	2.52	0.51
2:A:129:LYS:HG2	2:A:166:CYS:HB3	1.92	0.51
2:A:201:PHE:HB2	2:A:229:LEU:HD22	1.93	0.51
2:A:402:ILE:HG21	2:A:410:ILE:HG13	1.93	0.51
2:B:43:PHE:CE1	2:B:283:GLY:HA3	2.46	0.51
2:B:922:LEU:HD11	3:R:1:NAG:H5	1.93	0.51
2:C:287:ASP:HB3	2:C:306:PHE:HE2	1.74	0.51
2:C:973:ILE:HG21	2:C:983:ARG:HH22	1.76	0.51
2:C:406:GLU:OE1	2:C:495:TYR:OH	2.28	0.51
2:A:454:ARG:NH1	2:A:469:SER:O	2.44	0.51
2:A:656:VAL:HG22	2:A:693:ILE:HB	1.91	0.51
2:C:345:THR:HB	2:C:441:LEU:HD22	1.91	0.51
2:A:61:ASN:HD21	2:A:258:TRP:C	2.19	0.51
2:A:66:HIS:HA	2:A:263:ALA:HB1	1.93	0.51
2:B:191:GLU:HB2	2:B:223:LEU:HD21	1.92	0.51
2:B:544:ASN:C	2:B:546:LEU:H	2.18	0.51
2:C:736:VAL:HG22	2:C:767:LEU:HD12	1.93	0.51
2:A:105:ILE:HD11	2:A:116:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:TYR:OH	2:C:54:LEU:O	2.22	0.51
2:A:432:CYS:HB2	2:A:513:LEU:HG	1.92	0.50
2:A:1145:LEU:HD11	2:C:1145:LEU:HD12	1.93	0.50
2:B:119:ILE:HG23	2:B:128:ILE:HG23	1.92	0.50
2:B:1139:ASP:OD2	2:B:1142:GLN:N	2.42	0.50
2:A:244:LEU:O	2:A:246:ARG:N	2.44	0.50
2:B:601:GLY:O	2:B:602:THR:C	2.54	0.50
2:C:351:TYR:HA	2:C:353:TRP:CZ3	2.45	0.50
2:A:68:ILE:CD1	2:A:252:GLY:HA2	2.41	0.50
2:A:976:VAL:HG13	2:A:979:ASP:HB2	1.92	0.50
2:B:336:CYS:HB3	2:B:338:PHE:CE2	2.46	0.50
2:B:1077:THR:OG1	2:B:1078:ALA:N	2.43	0.50
1:I:72:SER:O	1:I:81:TYR:N	2.39	0.50
2:A:96:GLU:HB2	2:A:100:ILE:HB	1.93	0.50
2:A:139:PRO:HA	2:A:157:PHE:HA	1.92	0.50
2:B:270:LEU:H	2:B:270:LEU:HD12	1.77	0.50
2:B:1054:GLN:N	2:B:1061:VAL:O	2.43	0.50
2:C:327:VAL:O	2:C:530:SER:HB2	2.10	0.50
1:I:19:LEU:H	1:I:84:MET:HB2	1.77	0.50
2:A:703:ASN:O	2:C:789:TYR:HA	2.12	0.50
2:B:336:CYS:O	2:B:338:PHE:N	2.44	0.50
2:B:473:TYR:HB3	2:B:491:PRO:HD3	1.94	0.50
1:I:102:MET:HG3	1:I:105:LEU:HD22	1.94	0.50
2:A:290:ASP:OD1	2:A:291:CYS:N	2.42	0.50
2:A:724:THR:HB	2:A:934:ILE:HD11	1.93	0.50
2:C:106:PHE:HB2	2:C:117:LEU:HB2	1.93	0.50
2:C:581:THR:O	2:C:582:LEU:C	2.54	0.50
2:A:43:PHE:N	2:B:565:PHE:O	2.38	0.50
2:A:104:TRP:HB3	2:A:238:PHE:HE1	1.77	0.50
2:C:455:LEU:H	2:C:493:GLN:HE22	1.58	0.50
2:C:1115:ILE:HG22	2:C:1137:VAL:HG23	1.94	0.50
2:C:807:PRO:HG3	2:C:875:SER:HB2	1.92	0.50
2:A:551:VAL:N	2:A:588:THR:O	2.32	0.49
2:A:894:LEU:HD13	2:B:715:PRO:HD3	1.93	0.49
2:B:339:ASP:HA	2:B:343:ASN:HB2	1.94	0.49
2:B:401:VAL:O	2:B:495:TYR:OH	2.22	0.49
2:B:167:THR:HB	2:B:231:ILE:HD13	1.93	0.49
2:B:624:ILE:HG22	2:B:628:GLN:CG	2.42	0.49
2:B:1100:THR:OG1	2:B:1101:HIS:N	2.44	0.49
2:C:543:PHE:O	2:C:544:ASN:C	2.55	0.49
2:C:905:ARG:NH1	2:C:1049:LEU:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:592:PHE:HZ	2:C:857:GLY:H	1.60	0.49
2:B:43:PHE:HB3	2:C:566:GLY:HA2	1.92	0.49
2:B:347:PHE:HZ	2:B:511:VAL:HG22	1.78	0.49
2:B:770:ILE:HD11	2:B:1012:LEU:HA	1.93	0.49
2:B:864:LEU:HA	2:C:667:GLY:HA2	1.94	0.49
2:C:453:TYR:HB3	2:C:495:TYR:CE2	2.48	0.49
2:A:257:GLY:C	2:A:259:THR:N	2.68	0.49
2:A:677:GLN:O	2:A:689:SER:OG	2.24	0.49
2:C:393:THR:CA	2:C:522:ALA:HA	2.39	0.49
2:A:326:ILE:HD11	2:A:328:ARG:HB2	1.94	0.49
2:B:130:VAL:HG12	2:B:131:CYS:H	1.78	0.49
2:A:132:GLU:HB2	2:A:164:ASN:HB2	1.95	0.49
2:B:452:ARG:HG3	2:B:494:SER:HA	1.93	0.49
2:B:985:ASP:N	2:B:985:ASP:OD1	2.44	0.49
2:A:967:SER:N	2:B:571:ASP:OD2	2.46	0.49
2:B:789:TYR:HA	2:C:703:ASN:O	2.13	0.49
2:C:434:ILE:N	2:C:511:VAL:O	2.33	0.49
2:C:1077:THR:OG1	2:C:1078:ALA:N	2.44	0.49
2:A:448:ASN:HB3	2:A:497:PHE:HB2	1.93	0.49
2:B:905:ARG:HH11	2:B:905:ARG:HG2	1.76	0.49
2:C:111:ASP:OD2	2:C:113:LYS:NZ	2.34	0.49
2:B:63:THR:C	2:B:65:PHE:H	2.21	0.49
2:B:64:TRP:HB3	2:B:263:ALA:CB	2.42	0.49
2:A:350:VAL:HA	2:A:400:PHE:HB2	1.94	0.48
2:B:64:TRP:CZ3	2:B:266:TYR:HE1	2.31	0.48
2:B:759:PHE:HZ	2:C:1002:GLN:HG3	1.78	0.48
2:C:141:LEU:HD23	2:C:141:LEU:H	1.77	0.48
2:C:748:GLU:OE1	2:C:748:GLU:N	2.39	0.48
1:I:38:PHE:CD2	1:I:111:VAL:HG21	2.48	0.48
2:A:916:LEU:HD12	2:A:923:ILE:HD12	1.95	0.48
2:B:200:TYR:CE1	2:B:230:PRO:HB3	2.48	0.48
2:C:170:TYR:HE1	2:C:172:SER:HB2	1.77	0.48
2:C:322:PRO:HG3	2:C:549:THR:HG21	1.94	0.48
2:C:431:GLY:HA2	2:C:515:PHE:CD2	2.48	0.48
2:C:431:GLY:HA2	2:C:515:PHE:CE2	2.48	0.48
2:C:454:ARG:HD2	2:C:457:ARG:NH2	2.27	0.48
1:I:5:LEU:O	1:I:116:GLN:NE2	2.46	0.48
2:C:319:ARG:NH2	2:C:590:CYS:SG	2.86	0.48
2:C:392:PHE:HB3	2:C:515:PHE:HB3	1.95	0.48
2:A:563:GLN:HA	2:C:41:LYS:HB3	1.95	0.48
2:B:325:SER:HB2	2:B:539:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:TRP:HB2	2:C:66:HIS:NE2	2.28	0.48
2:A:814:LYS:HA	2:A:814:LYS:HD3	1.62	0.48
2:C:454:ARG:NH2	2:C:469:SER:O	2.47	0.48
1:I:31:THR:OG1	1:I:101:ASP:OD1	2.22	0.48
2:B:121:ASN:HA	2:B:126:VAL:HG12	1.95	0.48
2:C:115:GLN:HB2	2:C:233:ILE:HG12	1.96	0.48
2:C:170:TYR:CE1	2:C:172:SER:HB2	2.48	0.48
2:C:901:GLN:O	2:C:905:ARG:HG2	2.13	0.48
2:A:327:VAL:HG23	2:A:531:THR:CA	2.39	0.48
2:A:332:ILE:O	2:A:334:ASN:N	2.46	0.48
2:A:931:ILE:O	2:A:934:ILE:HG22	2.14	0.48
2:C:182:LYS:O	2:C:183:GLN:HG3	2.14	0.48
2:C:634:ARG:O	2:C:637:SER:OG	2.21	0.48
2:B:37:TYR:OH	2:B:195:LYS:NZ	2.46	0.48
2:C:1142:GLN:CD	2:C:1143:PRO:HD3	2.38	0.48
2:A:756:TYR:OH	2:A:998:THR:HG22	2.14	0.48
2:B:142:ASP:OD2	2:B:245:HIS:HA	2.14	0.48
2:B:654:GLU:OE1	2:B:654:GLU:N	2.47	0.48
2:A:543:PHE:O	2:A:546:LEU:HB2	2.14	0.47
2:A:1107:ARG:HG2	2:C:904:TYR:CE2	2.49	0.47
2:A:1138:TYR:HE1	2:A:1143:PRO:HG2	1.79	0.47
2:C:849:LEU:HD23	2:C:852:ALA:HB2	1.94	0.47
2:A:146:HIS:HD1	2:A:146:HIS:H	1.62	0.47
2:B:93:ALA:HA	2:B:190:ARG:O	2.13	0.47
2:B:624:ILE:HD11	2:B:637:SER:HA	1.96	0.47
2:B:1098:ASN:HD21	2:B:1101:HIS:HB2	1.78	0.47
2:C:65:PHE:CE2	2:C:82:PRO:HG2	2.49	0.47
2:A:232:GLY:HA3	4:A:1302:NAG:H62	1.96	0.47
2:A:434:ILE:HB	2:A:511:VAL:HB	1.96	0.47
2:B:759:PHE:CZ	2:C:1002:GLN:HG3	2.49	0.47
2:A:328:ARG:HD3	2:A:531:THR:OG1	2.14	0.47
2:B:804:GLN:NE2	2:B:935:GLN:OE1	2.30	0.47
2:C:335:LEU:HA	2:C:360:ASN:CA	2.39	0.47
2:C:973:ILE:HD11	2:C:992:GLN:HG3	1.97	0.47
2:B:118:LEU:O	2:B:120:VAL:HG13	2.14	0.47
2:B:280:ASN:OD1	2:B:281:GLU:HG3	2.13	0.47
2:A:68:ILE:HG13	2:A:78:ARG:C	2.40	0.47
2:A:257:GLY:O	2:A:258:TRP:C	2.58	0.47
2:A:375:PHE:HB3	2:A:436:TRP:HB3	1.96	0.47
2:A:393:THR:OG1	2:A:394:ASN:N	2.47	0.47
2:A:1028:LYS:NZ	2:A:1042:PHE:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1049:LEU:C	2:A:1050:MET:HG3	2.39	0.47
2:B:435:ALA:HA	2:B:509:ARG:O	2.14	0.47
2:A:58:PHE:C	2:A:60:SER:H	2.22	0.47
2:A:229:LEU:HD23	2:A:231:ILE:H	1.80	0.47
2:A:1029:MET:HE2	2:A:1029:MET:HB2	1.82	0.47
2:C:1146:ASP:O	2:C:1150:GLU:N	2.46	0.47
2:A:884:SER:O	2:A:887:THR:OG1	2.29	0.47
2:A:984:LEU:HB3	2:A:989:ALA:HB2	1.97	0.47
2:A:1082:CYS:HB2	2:A:1126:CYS:HB2	1.85	0.47
2:B:58:PHE:CE1	2:B:290:ASP:HB2	2.49	0.47
2:B:196:ASN:O	2:B:197:ILE:HD13	2.14	0.47
2:B:676:THR:HB	2:B:690:GLN:HG2	1.97	0.47
2:B:898:PHE:CE1	2:B:1050:MET:HE1	2.50	0.47
1:I:101:ASP:N	1:I:112:ASP:OD2	2.47	0.47
2:C:104:TRP:HE3	2:C:119:ILE:HB	1.79	0.47
2:C:167:THR:HG22	2:C:168:PHE:N	2.21	0.47
2:C:1050:MET:HE2	2:C:1052:PHE:CE1	2.49	0.47
2:A:120:VAL:HG22	2:A:157:PHE:HZ	1.80	0.46
2:B:318:PHE:CD1	2:B:629:LEU:HA	2.50	0.46
2:B:318:PHE:HD1	2:B:629:LEU:HA	1.80	0.46
2:B:497:PHE:CE1	2:B:507:PRO:HB3	2.50	0.46
2:C:38:TYR:CE1	2:C:224:GLU:HG3	2.50	0.46
2:C:97:LYS:HG2	2:C:100:ILE:HD11	1.97	0.46
1:I:65:VAL:HB	1:I:69:PHE:CD1	2.49	0.46
2:A:132:GLU:OE2	2:A:164:ASN:ND2	2.48	0.46
2:B:289:VAL:HG21	2:B:300:LYS:HD2	1.96	0.46
2:C:96:GLU:HB2	2:C:100:ILE:HB	1.97	0.46
2:A:106:PHE:HD2	2:A:235:ILE:HG21	1.80	0.46
2:A:244:LEU:HB3	2:A:247:SER:HB3	1.98	0.46
2:A:457:ARG:NH1	2:A:467:ASP:HB3	2.30	0.46
2:B:256:SER:O	2:B:258:TRP:N	2.48	0.46
2:B:722:VAL:HG22	2:B:1065:VAL:HG22	1.97	0.46
1:I:39:ARG:HG3	1:I:95:TYR:HD1	1.79	0.46
2:A:349:SER:HA	2:A:451:TYR:OH	2.15	0.46
2:A:534:VAL:HG21	2:A:539:VAL:HG21	1.97	0.46
2:A:898:PHE:O	2:A:899:PRO:C	2.56	0.46
2:B:359:SER:HB3	2:B:394:ASN:HA	1.98	0.46
2:B:596:SER:OG	2:B:613:GLN:OE1	2.27	0.46
2:C:193:VAL:HB	2:C:204:TYR:HB2	1.97	0.46
2:C:454:ARG:HE	2:C:491:PRO:HB2	1.80	0.46
2:A:107:GLY:N	2:A:235:ILE:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:SER:OG	2:B:117:LEU:N	2.49	0.46
2:B:294:ASP:OD1	2:B:295:PRO:HD2	2.15	0.46
2:A:131:CYS:HB2	2:A:166:CYS:HB3	1.55	0.46
2:A:767:LEU:HD23	2:A:767:LEU:HA	1.78	0.46
2:A:869:MET:HB2	2:B:699:LEU:HD21	1.98	0.46
2:B:1125:ASN:OD1	2:B:1125:ASN:N	2.39	0.46
2:C:368:LEU:H	2:C:368:LEU:HD23	1.80	0.46
2:C:412:PRO:HB3	2:C:427:ASP:HA	1.97	0.46
2:A:350:VAL:HG22	2:A:422:ASN:HB3	1.98	0.46
2:B:117:LEU:O	2:B:119:ILE:N	2.47	0.46
2:C:133:PHE:CE1	2:C:160:TYR:HB2	2.51	0.46
2:C:453:TYR:HB3	2:C:495:TYR:HE2	1.81	0.46
2:A:159:VAL:C	2:A:161:SER:H	2.24	0.46
2:A:170:TYR:OH	2:A:230:PRO:HD2	2.16	0.46
2:A:339:ASP:C	2:A:341:VAL:H	2.24	0.46
2:A:383:SER:O	2:A:387:LEU:N	2.49	0.46
2:B:36:VAL:HG11	2:B:220:PHE:CE2	2.51	0.46
2:C:157:PHE:CE2	2:C:159:VAL:HG13	2.51	0.46
2:C:177:MET:HE3	2:C:179:LEU:HD11	1.98	0.46
2:C:821:LEU:HD22	2:C:935:GLN:HG3	1.98	0.46
2:A:376:ALA:HB3	2:A:435:ALA:HB3	1.98	0.46
2:A:864:LEU:HA	2:B:667:GLY:HA2	1.98	0.46
2:B:878:LEU:O	2:B:882:ILE:HG12	2.15	0.46
2:A:72:GLY:N	2:A:78:ARG:O	2.49	0.46
2:A:326:ILE:HA	2:A:532:ASN:HD22	1.81	0.46
2:B:894:LEU:HD13	2:C:715:PRO:HD3	1.98	0.46
2:B:988:GLU:O	2:B:991:VAL:HG12	2.16	0.46
2:C:196:ASN:ND2	2:C:199:GLY:O	2.46	0.46
2:C:371:PHE:HZ	2:C:436:TRP:CE3	2.34	0.46
2:A:81:ASN:HD21	2:A:242:LEU:HD12	1.81	0.45
2:A:84:LEU:HD12	2:A:238:PHE:CD2	2.51	0.45
2:A:378:LYS:H	2:A:378:LYS:HG2	1.57	0.45
2:B:139:PRO:HA	2:B:157:PHE:HA	1.97	0.45
2:B:542:ASN:O	2:B:543:PHE:C	2.58	0.45
2:B:558:LYS:HE3	2:B:558:LYS:HB3	1.63	0.45
2:A:283:GLY:HA3	2:B:560:LEU:HD11	1.98	0.45
2:A:650:LEU:HD23	2:A:653:ALA:HB3	1.96	0.45
2:B:50:SER:HB2	2:B:276:LEU:HD12	1.98	0.45
2:C:276:LEU:HD22	2:C:301:CYS:HA	1.98	0.45
2:A:229:LEU:HD21	2:A:231:ILE:HB	1.99	0.45
2:C:391:CYS:HA	2:C:524:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:434:ILE:O	2:C:511:VAL:N	2.28	0.45
1:I:19:LEU:H	1:I:84:MET:CB	2.30	0.45
2:A:66:HIS:CE1	2:A:263:ALA:HA	2.51	0.45
2:A:589:PRO:HG3	2:C:855:PHE:HD1	1.80	0.45
2:B:234:ASN:OD1	2:B:234:ASN:N	2.49	0.45
2:C:282:ASN:HB2	2:C:284:THR:HG23	1.99	0.45
2:C:1050:MET:HE2	2:C:1052:PHE:CZ	2.52	0.45
2:A:339:ASP:C	2:A:341:VAL:N	2.74	0.45
2:B:64:TRP:CH2	2:B:266:TYR:HE1	2.35	0.45
2:B:121:ASN:ND2	2:B:176:LEU:HB2	2.32	0.45
2:B:523:THR:O	2:B:525:CYS:N	2.46	0.45
2:B:600:PRO:HB3	2:B:674:TYR:HB2	1.99	0.45
2:B:712:ILE:O	2:B:1075:PHE:N	2.49	0.45
1:I:75:ASN:ND2	2:C:501:TYR:O	2.46	0.45
2:A:97:LYS:H	2:A:100:ILE:HD13	1.82	0.45
2:A:372:ALA:HB3	2:A:375:PHE:HD2	1.81	0.45
2:A:525:CYS:O	2:A:526:GLY:C	2.59	0.45
2:A:624:ILE:HD11	2:A:637:SER:HA	1.99	0.45
2:A:1054:GLN:N	2:A:1061:VAL:O	2.48	0.45
2:B:78:ARG:O	2:B:79:PHE:C	2.59	0.45
2:B:200:TYR:HB2	2:B:202:LYS:HE3	1.99	0.45
2:B:616:ASN:HB3	2:B:619:GLU:HG3	1.98	0.45
2:C:393:THR:HB	2:C:522:ALA:HA	1.98	0.45
2:C:435:ALA:HB2	2:C:510:VAL:HG13	1.98	0.45
2:C:630:THR:OG1	2:C:631:PRO:HD3	2.17	0.45
2:A:30:ASN:HA	2:A:61:ASN:CB	2.45	0.45
2:A:792:PRO:HG2	2:B:707:TYR:HB3	1.98	0.45
2:B:137:ASN:HB2	2:B:159:VAL:CA	2.35	0.45
2:B:277:LEU:HD23	2:B:285:ILE:HD13	1.98	0.45
2:C:573:THR:O	2:C:573:THR:OG1	2.30	0.45
2:A:351:TYR:HB2	2:A:454:ARG:HH21	1.82	0.45
2:A:442:ASP:O	2:A:448:ASN:ND2	2.50	0.45
2:A:462:LYS:HA	2:A:462:LYS:HD3	1.83	0.45
2:A:709:ASN:OD1	2:A:709:ASN:N	2.50	0.45
2:A:929:SER:O	2:A:933:LYS:HG2	2.17	0.45
2:C:419:ALA:O	2:C:424:LYS:NZ	2.49	0.45
2:C:1096:VAL:HG21	2:C:1110:TYR:HE1	1.82	0.45
1:I:69:PHE:CZ	1:I:84:MET:HE1	2.52	0.45
2:A:39:PRO:HG3	2:A:51:THR:HG21	1.99	0.45
2:A:52:GLN:HA	2:A:274:THR:HA	1.99	0.45
2:A:598:ILE:N	2:A:609:ALA:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:THR:O	2:B:237:ARG:HG2	2.17	0.45
2:B:1035:GLY:HA3	2:C:1040:VAL:HG21	1.98	0.45
2:C:902:MET:HE1	2:C:1050:MET:SD	2.56	0.45
2:C:986:PRO:N	2:C:987:PRO:HD2	2.32	0.45
2:A:444:LYS:H	2:A:448:ASN:HB2	1.82	0.44
2:A:821:LEU:HD13	2:A:935:GLN:HG3	1.98	0.44
2:C:802:PHE:HD1	2:C:805:ILE:HD11	1.82	0.44
2:C:1082:CYS:HB2	2:C:1126:CYS:HB2	1.93	0.44
1:I:39:ARG:HG2	1:I:40:GLN:N	2.31	0.44
2:B:560:LEU:O	2:B:577:ARG:NH2	2.49	0.44
2:C:289:VAL:HG21	2:C:300:LYS:HD2	1.97	0.44
2:C:328:ARG:NH1	2:C:328:ARG:CG	2.77	0.44
2:C:543:PHE:HD2	2:C:579:PRO:HD3	1.82	0.44
2:C:580:GLN:C	2:C:582:LEU:H	2.25	0.44
1:I:94:THR:OG1	1:I:119:GLN:OE1	2.34	0.44
2:A:92:PHE:CD1	2:A:92:PHE:C	2.95	0.44
2:A:295:PRO:HG3	2:A:633:TRP:CE2	2.52	0.44
2:A:631:PRO:O	2:A:632:THR:OG1	2.30	0.44
2:C:111:ASP:OD1	2:C:114:THR:OG1	2.32	0.44
2:C:220:PHE:HE2	2:C:285:ILE:HG22	1.82	0.44
2:A:650:LEU:HD11	2:A:666:ILE:HD13	1.98	0.44
2:A:708:SER:OG	2:A:709:ASN:N	2.50	0.44
2:A:789:TYR:HA	2:B:703:ASN:O	2.16	0.44
2:A:904:TYR:OH	2:B:1094:VAL:HB	2.18	0.44
2:B:80:ASP:HB3	2:B:81:ASN:H	1.63	0.44
2:B:216:LEU:HG	2:B:266:TYR:OH	2.16	0.44
2:B:598:ILE:HG23	2:B:664:ILE:HG21	1.99	0.44
2:C:393:THR:OG1	2:C:394:ASN:N	2.50	0.44
2:C:433:VAL:HG12	2:C:512:VAL:HG22	1.99	0.44
2:C:474:GLN:HA	2:C:488:CYS:SG	2.57	0.44
2:C:580:GLN:C	2:C:582:LEU:N	2.76	0.44
1:I:40:GLN:H	1:I:40:GLN:CD	2.26	0.44
2:A:105:ILE:HB	2:A:241:LEU:HD21	1.98	0.44
2:A:1097:SER:HB3	2:A:1102:TRP:CD2	2.52	0.44
2:A:207:HIS:CD2	2:A:209:PRO:HD3	2.52	0.44
2:A:435:ALA:HA	2:A:509:ARG:O	2.18	0.44
4:A:1307:NAG:H61	2:C:794:ILE:HG12	1.98	0.44
2:B:743:CYS:HB3	2:B:749:CYS:HB3	1.82	0.44
2:C:96:GLU:OE1	2:C:100:ILE:N	2.50	0.44
2:C:546:LEU:HD11	2:C:565:PHE:CE1	2.53	0.44
2:C:767:LEU:HD23	2:C:767:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:969:LYS:HE3	2:C:974:SER:HA	1.98	0.44
2:A:280:ASN:N	2:A:284:THR:O	2.37	0.44
2:B:189:LEU:HD21	2:B:212:LEU:HD13	1.99	0.44
2:C:392:PHE:HD1	2:C:517:LEU:HD11	1.81	0.44
2:A:131:CYS:SG	2:A:163:ALA:O	2.76	0.44
2:A:714:ILE:HD11	2:A:1094:VAL:HG11	1.99	0.44
2:B:58:PHE:HE1	2:B:290:ASP:HB2	1.83	0.44
2:B:202:LYS:HA	2:B:228:ASP:HA	1.99	0.44
2:B:767:LEU:HD23	2:B:767:LEU:HA	1.82	0.44
2:C:281:GLU:C	2:C:283:GLY:H	2.24	0.44
2:A:77:LYS:NZ	2:A:80:ASP:HB3	2.33	0.44
2:A:112:SER:HA	2:A:132:GLU:HG2	2.00	0.44
2:A:715:PRO:HA	2:A:1072:GLU:HA	2.00	0.44
2:B:204:TYR:HA	2:B:225:PRO:HA	1.99	0.44
2:B:462:LYS:HA	2:B:462:LYS:HD3	1.71	0.44
2:C:233:ILE:HD12	2:C:233:ILE:HA	1.93	0.44
2:C:350:VAL:HG21	2:C:418:ILE:CG1	2.42	0.44
1:I:17:GLY:O	1:I:87:LEU:N	2.44	0.43
2:A:177:MET:H	2:A:177:MET:HG3	1.68	0.43
2:A:433:VAL:HG13	2:A:510:VAL:HG13	2.00	0.43
2:A:1002:GLN:C	2:A:1002:GLN:OE1	2.61	0.43
2:C:811:LYS:HE3	2:C:811:LYS:HB2	1.65	0.43
1:I:15:PRO:HB3	1:I:89:ALA:HB2	2.00	0.43
1:I:28:TRP:HB3	2:C:375:PHE:HE1	1.83	0.43
2:A:788:ILE:HG23	2:A:876:ALA:HB2	1.99	0.43
2:B:294:ASP:H	2:B:297:SER:HB2	1.83	0.43
2:B:1094:VAL:HG13	2:B:1096:VAL:HG13	2.00	0.43
2:C:126:VAL:HG13	2:C:174:PRO:HA	2.00	0.43
2:C:601:GLY:O	2:C:602:THR:C	2.61	0.43
2:C:762:GLN:HE22	2:C:765:ARG:NH1	2.16	0.43
2:C:1029:MET:HE2	2:C:1053:PRO:HB3	2.00	0.43
2:A:222:ALA:HB2	2:A:285:ILE:HB	2.00	0.43
2:A:462:LYS:HB2	2:A:465:GLU:HB2	1.99	0.43
2:A:566:GLY:HA2	2:C:43:PHE:H	1.84	0.43
2:A:877:LEU:HD12	2:A:877:LEU:HA	1.87	0.43
2:A:898:PHE:HB3	2:A:899:PRO:HD3	2.00	0.43
2:A:919:ASN:O	2:A:923:ILE:HG13	2.18	0.43
2:A:1073:LYS:HE2	2:A:1073:LYS:HB3	1.38	0.43
2:C:849:LEU:HG	2:C:851:CYS:N	2.31	0.43
2:A:328:ARG:NH1	2:A:578:ASP:OD2	2.51	0.43
2:A:394:ASN:OD1	2:A:394:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:997:ILE:HD13	2:A:997:ILE:HA	1.77	0.43
2:B:1126:CYS:SG	2:B:1126:CYS:O	2.76	0.43
2:C:244:LEU:HG	2:C:246:ARG:H	1.84	0.43
2:C:290:ASP:O	2:C:297:SER:HB3	2.18	0.43
2:C:418:ILE:HA	2:C:422:ASN:HB2	2.00	0.43
2:C:441:LEU:HD23	2:C:441:LEU:HA	1.78	0.43
2:C:599:THR:HB	2:C:608:VAL:HG12	1.99	0.43
1:I:53:ASP:OD2	1:I:57:THR:OG1	2.24	0.43
2:A:94:SER:HB2	2:A:265:TYR:HB2	1.99	0.43
2:A:106:PHE:HB3	2:A:235:ILE:HG23	2.00	0.43
2:A:432:CYS:N	2:A:513:LEU:O	2.48	0.43
2:B:320:VAL:HA	2:B:628:GLN:OE1	2.18	0.43
2:B:330:PRO:HA	2:B:579:PRO:CB	2.36	0.43
2:B:978:ASN:O	2:B:981:LEU:HG	2.19	0.43
2:A:150:LYS:HA	2:A:150:LYS:HD2	1.75	0.43
2:B:37:TYR:HB3	2:B:223:LEU:HB2	2.01	0.43
2:B:622:VAL:HG21	2:B:642:VAL:HG11	2.01	0.43
2:C:531:THR:HB	2:C:532:ASN:H	1.54	0.43
2:C:850:ILE:HG22	2:C:854:LYS:HE3	2.00	0.43
2:C:1097:SER:C	2:C:1099:GLY:H	2.27	0.43
2:A:65:PHE:CE1	2:A:67:ALA:HB2	2.54	0.43
2:A:130:VAL:HB	2:A:167:THR:HB	2.00	0.43
2:C:189:LEU:HD12	2:C:208:THR:HG21	2.00	0.43
2:C:356:LYS:HD2	2:C:356:LYS:HA	1.81	0.43
1:I:53:ASP:CG	1:I:57:THR:H	2.26	0.43
1:I:73:ARG:HE	2:C:503:VAL:HG11	1.83	0.43
2:B:156:GLU:OE2	2:B:245:HIS:HB2	2.19	0.43
2:B:160:TYR:HD2	2:B:160:TYR:H	1.64	0.43
2:B:1012:LEU:HA	2:B:1012:LEU:HD23	1.83	0.43
2:C:167:THR:HG22	2:C:168:PHE:HD1	1.84	0.43
2:A:126:VAL:CG2	2:A:174:PRO:HA	2.49	0.43
2:A:393:THR:HB	2:A:520:ALA:HB3	2.00	0.43
2:A:442:ASP:OD2	2:A:509:ARG:NE	2.39	0.43
2:A:669:GLY:HA3	2:C:869:MET:HE1	1.99	0.43
2:B:110:LEU:HD12	2:B:136:CYS:HB3	2.01	0.43
2:A:129:LYS:HD2	2:A:169:GLU:HB2	2.01	0.43
2:A:426:PRO:HG2	2:A:429:PHE:HB2	2.00	0.43
2:A:707:TYR:HB3	2:C:792:PRO:HG2	2.01	0.43
2:B:329:PHE:N	2:B:330:PRO:HD3	2.34	0.43
2:B:434:ILE:O	2:B:510:VAL:HA	2.19	0.43
2:B:633:TRP:C	2:B:635:VAL:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:650:LEU:HD12	2:B:650:LEU:HA	1.82	0.43
2:B:802:PHE:CD1	2:B:805:ILE:HD11	2.54	0.43
2:B:1030:SER:O	2:B:1034:LEU:HB2	2.18	0.43
2:C:143:VAL:HG22	2:C:144:TYR:N	2.34	0.43
2:A:582:LEU:HD22	2:A:582:LEU:HA	1.67	0.42
2:A:811:LYS:HE3	2:A:811:LYS:HB2	1.81	0.42
2:A:905:ARG:HD2	2:A:1050:MET:HG2	2.00	0.42
2:B:48:LEU:HD13	2:B:48:LEU:HA	1.82	0.42
2:B:137:ASN:CG	2:B:159:VAL:HA	2.43	0.42
2:B:742:ILE:HG23	2:B:997:ILE:HD12	2.00	0.42
2:C:278:LYS:HD3	2:C:286:THR:HB	2.01	0.42
2:C:655:TYR:HE2	4:C:1306:NAG:H81	1.83	0.42
1:I:19:LEU:HD13	1:I:84:MET:HE3	2.01	0.42
2:A:1035:GLY:HA3	2:B:1040:VAL:HG21	2.00	0.42
2:B:86:PHE:O	2:B:86:PHE:CD1	2.72	0.42
2:B:1116:THR:HA	2:B:1138:TYR:O	2.19	0.42
2:A:900:MET:HE2	2:A:900:MET:HB3	1.79	0.42
2:B:347:PHE:CZ	2:B:399:SER:HB2	2.54	0.42
2:B:591:SER:OG	2:B:620:VAL:HG21	2.19	0.42
2:C:328:ARG:NH2	2:C:543:PHE:CG	2.86	0.42
2:C:334:ASN:ND2	2:C:361:CYS:O	2.52	0.42
2:C:409:GLN:NE2	2:C:416:GLY:HA3	2.34	0.42
2:C:421:TYR:HB3	2:C:457:ARG:HD2	2.01	0.42
2:C:458:LYS:HB2	2:C:473:TYR:HE1	1.84	0.42
2:C:543:PHE:CD2	2:C:579:PRO:HD3	2.54	0.42
2:A:326:ILE:HG23	2:A:541:PHE:HA	2.02	0.42
2:A:748:GLU:H	2:A:748:GLU:CD	2.27	0.42
2:A:849:LEU:HD21	2:A:852:ALA:HB3	2.01	0.42
2:B:29:THR:OG1	2:B:30:ASN:N	2.52	0.42
2:B:56:LEU:HD12	2:B:56:LEU:HA	1.73	0.42
2:B:175:PHE:HB3	2:B:226:LEU:HD23	2.00	0.42
2:B:177:MET:HG3	2:B:207:HIS:ND1	2.34	0.42
2:C:287:ASP:HB3	2:C:306:PHE:CE2	2.53	0.42
2:C:756:TYR:HB3	2:C:759:PHE:CD2	2.54	0.42
2:C:978:ASN:OD1	2:C:978:ASN:N	2.46	0.42
2:A:490:PHE:CE2	2:A:492:LEU:HB2	2.55	0.42
2:A:719:THR:N	2:A:1068:VAL:O	2.52	0.42
2:A:905:ARG:HD2	2:A:1050:MET:CG	2.50	0.42
2:B:433:VAL:HG12	2:B:512:VAL:HA	2.01	0.42
2:B:998:THR:O	2:B:1001:LEU:HD23	2.19	0.42
2:B:1048:HIS:HE2	2:B:1050:MET:C	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:TRP:NE1	2:C:369:TYR:HB3	2.32	0.42
2:A:426:PRO:HB3	2:A:463:PRO:HB3	2.00	0.42
2:B:258:TRP:CB	4:B:1302:NAG:H5	2.48	0.42
2:B:300:LYS:HB2	2:B:305:SER:O	2.20	0.42
2:B:338:PHE:CD1	2:B:342:PHE:HE2	2.31	0.42
2:C:33:THR:OG1	2:C:219:GLY:O	2.25	0.42
1:I:74:ASP:HB2	1:I:81:TYR:CE2	2.54	0.42
2:A:263:ALA:HB3	2:A:266:TYR:CE2	2.54	0.42
2:B:75:GLY:O	2:B:76:THR:C	2.63	0.42
2:B:140:PHE:H	2:B:157:PHE:HA	1.84	0.42
2:B:785:VAL:HG12	2:B:787:GLN:H	1.83	0.42
2:A:191:GLU:O	2:A:223:LEU:HD21	2.19	0.42
2:A:635:VAL:HG13	2:A:636:TYR:CD1	2.50	0.42
2:A:764:LYS:O	2:A:768:THR:HG23	2.19	0.42
2:B:84:LEU:O	2:B:237:ARG:HA	2.20	0.42
2:B:156:GLU:OE1	2:B:245:HIS:N	2.53	0.42
2:B:393:THR:HA	2:B:521:PRO:HA	2.01	0.42
2:B:577:ARG:HH11	2:B:582:LEU:HG	1.84	0.42
2:B:773:GLU:HG3	2:B:1019:ARG:HH21	1.84	0.42
2:B:819:GLU:OE2	2:B:1055:SER:OG	2.31	0.42
2:B:946:GLY:O	2:B:950:ASP:HB2	2.19	0.42
2:C:38:TYR:CE2	2:C:285:ILE:HG13	2.55	0.42
1:I:34:HIS:HB3	1:I:52:ILE:O	2.20	0.42
2:A:336:CYS:SG	2:A:362:VAL:N	2.92	0.42
2:A:546:LEU:HD23	2:A:546:LEU:HA	1.80	0.42
2:A:828:LEU:HB2	2:A:850:ILE:HD13	2.00	0.42
2:B:117:LEU:O	2:B:119:ILE:HG13	2.20	0.42
2:B:157:PHE:HD2	2:B:159:VAL:HG23	1.84	0.42
2:B:199:GLY:O	2:B:231:ILE:N	2.42	0.42
2:B:1005:GLN:NE2	2:C:1002:GLN:HE22	2.17	0.42
2:C:86:PHE:HB2	2:C:238:PHE:HB3	2.02	0.42
2:A:202:LYS:HD2	2:A:202:LYS:HA	1.66	0.42
2:A:541:PHE:HB3	2:A:552:LEU:HD11	2.02	0.42
2:B:66:HIS:CE1	2:B:263:ALA:HA	2.55	0.42
2:B:99:ASN:OD1	2:B:102:ARG:HD2	2.19	0.42
2:B:454:ARG:HG3	2:B:491:PRO:HB2	2.02	0.42
2:B:802:PHE:HD1	2:B:805:ILE:HD11	1.85	0.42
2:C:57:PRO:O	2:C:60:SER:HB3	2.20	0.42
2:C:310:LYS:HD2	2:C:663:ASP:OD2	2.20	0.42
2:C:1125:ASN:OD1	2:C:1126:CYS:N	2.52	0.42
2:A:63:THR:HA	2:A:257:GLY:CA	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:167:THR:HG23	2:B:357:ARG:HH21	1.85	0.41
2:A:325:SER:HA	2:A:540:ASN:OD1	2.20	0.41
2:A:617:CYS:CA	2:A:621:PRO:HD2	2.50	0.41
2:A:1123:SER:O	2:A:1123:SER:OG	2.29	0.41
2:B:540:ASN:OD1	2:B:549:THR:OG1	2.37	0.41
2:C:102:ARG:HD3	2:C:121:ASN:O	2.20	0.41
2:A:295:PRO:HG3	2:A:633:TRP:CZ2	2.54	0.41
2:C:335:LEU:HD13	2:C:525:CYS:H	1.84	0.41
2:C:708:SER:HB3	2:C:711:SER:HB3	2.02	0.41
2:C:748:GLU:HG2	2:C:749:CYS:N	2.36	0.41
2:A:36:VAL:O	2:A:223:LEU:HB2	2.21	0.41
2:A:390:LEU:HD23	2:A:390:LEU:HA	1.80	0.41
2:A:763:LEU:HD13	2:A:1004:LEU:HG	2.01	0.41
2:B:336:CYS:O	2:B:337:PRO:C	2.63	0.41
2:C:100:ILE:H	2:C:100:ILE:HG13	1.64	0.41
2:A:1074:ASN:OD1	2:A:1074:ASN:N	2.51	0.41
2:A:1138:TYR:CE1	2:A:1143:PRO:HG2	2.54	0.41
2:B:37:TYR:HA	2:B:223:LEU:H	1.84	0.41
2:B:428:ASP:OD1	2:B:428:ASP:N	2.50	0.41
2:B:441:LEU:HD23	2:B:441:LEU:HA	1.87	0.41
2:B:535:LYS:HZ2	2:B:535:LYS:C	2.26	0.41
2:B:752:LEU:HD23	2:B:993:ILE:HG22	2.03	0.41
2:B:959:LEU:HD23	2:B:959:LEU:HA	1.85	0.41
2:C:354:ASN:ND2	2:C:356:LYS:HG2	2.35	0.41
2:A:126:VAL:O	2:A:171:VAL:HA	2.20	0.41
2:B:42:VAL:O	2:C:563:GLN:NE2	2.42	0.41
2:B:92:PHE:O	2:B:192:PHE:N	2.53	0.41
2:C:442:ASP:O	2:C:448:ASN:ND2	2.53	0.41
2:C:461:LEU:HD13	2:C:465:GLU:C	2.44	0.41
2:C:643:PHE:CE2	2:C:645:THR:HG22	2.55	0.41
2:A:64:TRP:HB2	2:A:259:THR:O	2.20	0.41
2:A:894:LEU:HB3	2:B:713:ALA:HB3	2.03	0.41
2:A:959:LEU:HD12	2:A:959:LEU:HA	1.84	0.41
2:B:64:TRP:O	2:B:66:HIS:N	2.54	0.41
2:B:775:ASP:OD1	2:B:864:LEU:HB3	2.21	0.41
2:C:261:GLY:O	2:C:266:TYR:OH	2.35	0.41
2:A:68:ILE:HD13	2:A:252:GLY:HA2	2.01	0.41
2:A:182:LYS:HD3	2:A:182:LYS:N	2.35	0.41
2:B:137:ASN:N	2:B:159:VAL:HG22	2.35	0.41
2:B:760:CYS:HA	2:B:763:LEU:HG	2.03	0.41
2:C:244:LEU:C	2:C:246:ARG:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:376:ALA:N	2:C:435:ALA:O	2.44	0.41
1:I:65:VAL:HB	1:I:69:PHE:CG	2.55	0.41
1:I:82:LEU:HD12	1:I:82:LEU:HA	1.97	0.41
2:A:276:LEU:HD13	2:A:304:LYS:HZ2	1.85	0.41
2:A:903:ALA:HB2	2:A:916:LEU:HD23	2.02	0.41
2:B:29:THR:N	2:B:62:VAL:O	2.53	0.41
2:B:32:PHE:O	2:B:58:PHE:HB3	2.21	0.41
2:B:331:ASN:O	2:B:580:GLN:HB2	2.21	0.41
2:B:993:ILE:HD13	2:B:993:ILE:HA	1.94	0.41
2:C:36:VAL:HG21	2:C:220:PHE:CZ	2.55	0.41
2:C:92:PHE:HB3	2:C:192:PHE:HB2	2.02	0.41
2:C:434:ILE:HG12	2:C:513:LEU:HD11	2.03	0.41
2:C:472:ILE:HD12	2:C:484:ALA:HB2	2.02	0.41
2:A:181:GLY:HA3	2:A:186:PHE:CD1	2.56	0.41
2:A:242:LEU:HD23	2:A:242:LEU:HA	1.79	0.41
2:A:363:ALA:O	2:A:364:ASP:C	2.62	0.41
2:A:534:VAL:HG22	2:A:535:LYS:H	1.85	0.41
2:A:741:TYR:CE1	2:A:966:LEU:HD21	2.56	0.41
2:B:99:ASN:O	2:B:100:ILE:C	2.64	0.41
2:C:280:ASN:CG	2:C:284:THR:HG1	2.27	0.41
2:C:434:ILE:HB	2:C:511:VAL:HB	2.01	0.41
2:C:650:LEU:HD12	2:C:650:LEU:HA	1.80	0.41
2:C:1102:TRP:CZ2	2:C:1133:VAL:HG11	2.56	0.41
2:A:30:ASN:HA	2:A:61:ASN:CA	2.49	0.41
2:B:337:PRO:HB2	2:B:358:ILE:HD13	2.02	0.41
2:B:624:ILE:HG22	2:B:628:GLN:HG2	2.02	0.41
2:B:931:ILE:O	2:B:934:ILE:HG22	2.21	0.41
2:C:403:ARG:HG3	2:C:405:ASN:H	1.85	0.41
2:A:141:LEU:HD23	2:A:141:LEU:HA	1.88	0.40
2:B:135:PHE:O	2:B:159:VAL:HG13	2.21	0.40
2:B:636:TYR:HB3	2:B:651:ILE:HG21	2.02	0.40
2:B:993:ILE:O	2:B:997:ILE:HG12	2.21	0.40
2:C:959:LEU:HD12	2:C:959:LEU:HA	1.77	0.40
1:I:51:ALA:HB3	1:I:60:TYR:HB2	2.03	0.40
2:A:339:ASP:O	2:A:341:VAL:N	2.54	0.40
2:A:403:ARG:HD2	2:A:505:HIS:HA	2.03	0.40
2:A:457:ARG:HG2	2:A:458:LYS:H	1.87	0.40
2:A:733:LYS:HB3	2:A:861:LEU:HB2	2.03	0.40
2:B:156:GLU:HB2	2:B:158:ARG:NH1	2.36	0.40
2:B:416:GLY:O	2:B:420:ASP:HB2	2.21	0.40
2:B:433:VAL:O	2:B:433:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:866:THR:HG23	2:B:869:MET:H	1.85	0.40
2:C:964:LYS:HD3	2:C:964:LYS:HA	1.88	0.40
2:A:973:ILE:HG22	2:A:983:ARG:HH21	1.87	0.40
2:A:1051:SER:OG	2:A:1064:HIS:ND1	2.41	0.40
2:A:1094:VAL:CG2	2:C:900:MET:HE1	2.46	0.40
2:B:83:VAL:CG2	2:B:237:ARG:HE	2.25	0.40
2:B:115:GLN:HA	2:B:132:GLU:H	1.87	0.40
2:B:197:ILE:O	2:B:202:LYS:NZ	2.54	0.40
2:C:230:PRO:O	2:C:231:ILE:C	2.65	0.40
2:C:615:VAL:H	2:C:648:GLY:HA2	1.86	0.40
2:C:849:LEU:HD11	2:C:851:CYS:HB2	2.02	0.40
2:C:1052:PHE:HB2	2:C:1063:LEU:HB2	2.03	0.40
2:C:1080:ALA:O	2:C:1132:ILE:HG13	2.21	0.40
2:A:273:ARG:HD3	2:A:273:ARG:HA	1.58	0.40
2:A:645:THR:HG22	2:A:647:ALA:N	2.27	0.40
2:B:602:THR:O	2:B:603:ASN:C	2.64	0.40
2:A:425:LEU:HD23	2:A:425:LEU:HA	1.97	0.40
2:B:331:ASN:HB3	2:B:580:GLN:HG2	2.04	0.40
2:B:336:CYS:HB2	2:B:361:CYS:HB3	1.12	0.40
2:B:826:VAL:HG23	2:B:945:LEU:HD22	2.03	0.40
2:C:311:GLY:HA2	2:C:664:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	123/124 (99%)	117 (95%)	6 (5%)	0	100 100
2	A	1075/1288 (84%)	962 (90%)	100 (9%)	13 (1%)	10 42
2	B	1074/1288 (83%)	935 (87%)	118 (11%)	21 (2%)	6 32
2	C	1076/1288 (84%)	967 (90%)	92 (9%)	17 (2%)	7 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3348/3988 (84%)	2981 (89%)	316 (9%)	51 (2%)	11 37

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	337	PRO
2	A	602	THR
2	A	603	ASN
2	B	65	PHE
2	B	74	ASN
2	B	117	LEU
2	B	332	ILE
2	B	710	ASN
2	C	231	ILE
2	C	330	PRO
2	C	340	GLU
2	C	361	CYS
2	A	63	THR
2	A	245	HIS
2	A	340	GLU
2	B	160	TYR
2	B	254	SER
2	B	257	GLY
2	B	524	VAL
2	B	583	GLU
2	B	634	ARG
2	C	338	PHE
2	C	342	PHE
2	C	346	ARG
2	C	581	THR
2	C	582	LEU
2	A	112	SER
2	A	115	GLN
2	A	166	CYS
2	A	332	ILE
2	A	333	THR
2	B	73	THR
2	B	132	GLU
2	B	133	PHE
2	B	337	PRO
2	C	543	PHE
2	B	163	ALA

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Mol	Chain	Res	Type
2	B	233	ILE
2	B	582	LEU
2	C	331	ASN
2	C	441	LEU
2	C	534	VAL
2	B	118	LEU
2	B	166	CYS
2	C	362	VAL
2	A	160	TYR
2	B	256	SER
2	C	329	PHE
2	C	341	VAL
2	C	337	PRO
2	A	534	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	102/101 (101%)	102 (100%)	0	100	100
2	A	925/1113 (83%)	886 (96%)	39 (4%)	26	52
2	B	933/1113 (84%)	877 (94%)	56 (6%)	17	44
2	C	935/1113 (84%)	885 (95%)	50 (5%)	20	47
All	All	2895/3440 (84%)	2750 (95%)	145 (5%)	23	49

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	36	VAL
2	A	61	ASN
2	A	62	VAL
2	A	66	HIS
2	A	68	ILE
2	A	73	THR
2	A	108	THR

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Mol	Chain	Res	Type
2	A	111	ASP
2	A	113	LYS
2	A	129	LYS
2	A	132	GLU
2	A	161	SER
2	A	165	ASN
2	A	167	THR
2	A	189	LEU
2	A	236	THR
2	A	249	LEU
2	A	250	THR
2	A	259	THR
2	A	280	ASN
2	A	281	GLU
2	A	309	GLU
2	A	335	LEU
2	A	361	CYS
2	A	525	CYS
2	A	531	THR
2	A	533	LEU
2	A	582	LEU
2	A	656	VAL
2	A	658	SER
2	A	659	SER
2	A	708	SER
2	A	709	ASN
2	A	740	MET
2	A	795	LYS
2	A	896	ILE
2	A	1005	GLN
2	A	1073	LYS
2	A	1074	ASN
2	B	29	THR
2	B	61	ASN
2	B	62	VAL
2	B	63	THR
2	B	76	THR
2	B	77	LYS
2	B	79	PHE
2	B	90	VAL
2	B	95	THR
2	B	96	GLU

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Mol	Chain	Res	Type
2	B	101	ILE
2	B	111	ASP
2	B	112	SER
2	B	113	LYS
2	B	117	LEU
2	B	118	LEU
2	B	128	ILE
2	B	129	LYS
2	B	130	VAL
2	B	135	PHE
2	B	164	ASN
2	B	165	ASN
2	B	166	CYS
2	B	167	THR
2	B	233	ILE
2	B	235	ILE
2	B	247	SER
2	B	255	SER
2	B	259	THR
2	B	329	PHE
2	B	361	CYS
2	B	362	VAL
2	B	375	PHE
2	B	377	PHE
2	B	524	VAL
2	B	525	CYS
2	B	544	ASN
2	B	558	LYS
2	B	581	THR
2	B	583	GLU
2	B	605	SER
2	B	619	GLU
2	B	624	ILE
2	B	633	TRP
2	B	635	VAL
2	B	712	ILE
2	B	931	ILE
2	B	933	LYS
2	B	1081	ILE
2	B	1097	SER
2	B	1114	ILE
2	B	1115	ILE

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Mol	Chain	Res	Type
2	B	1116	THR
2	B	1118	ASP
2	B	1119	ASN
2	B	1136	THR
2	C	68	ILE
2	C	73	THR
2	C	80	ASP
2	C	177	MET
2	C	234	ASN
2	C	236	THR
2	C	280	ASN
2	C	284	THR
2	C	328	ARG
2	C	329	PHE
2	C	332	ILE
2	C	335	LEU
2	C	338	PHE
2	C	340	GLU
2	C	341	VAL
2	C	343	ASN
2	C	345	THR
2	C	350	VAL
2	C	358	ILE
2	C	364	ASP
2	C	365	TYR
2	C	369	TYR
2	C	370	ASN
2	C	371	PHE
2	C	387	LEU
2	C	389	ASP
2	C	393	THR
2	C	440	LYS
2	C	461	LEU
2	C	462	LYS
2	C	468	ILE
2	C	524	VAL
2	C	525	CYS
2	C	531	THR
2	C	533	LEU
2	C	534	VAL
2	C	544	ASN
2	C	577	ARG

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Mol	Chain	Res	Type
2	C	580	GLN
2	C	602	THR
2	C	657	ASN
2	C	747	THR
2	C	875	SER
2	C	978	ASN
2	C	1072	GLU
2	C	1073	LYS
2	C	1097	SER
2	C	1104	VAL
2	C	1111	GLU
2	C	1133	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	66	HIS
2	A	207	HIS
2	A	321	GLN
2	A	334	ASN
2	A	370	ASN
2	A	532	ASN
2	A	901	GLN
2	A	914	ASN
2	A	1005	GLN
2	A	1142	GLN
2	B	52	GLN
2	B	81	ASN
2	B	121	ASN
2	B	165	ASN
2	B	343	ASN
2	B	422	ASN
2	B	437	ASN
2	B	439	ASN
2	B	519	HIS
2	B	564	GLN
2	B	628	GLN
2	B	784	GLN
2	B	919	ASN
2	B	954	HIS
2	B	960	ASN
2	B	1005	GLN

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Mol	Chain	Res	Type
2	B	1011	GLN
2	B	1119	ASN
2	C	87	ASN
2	C	121	ASN
2	C	211	ASN
2	C	271	GLN
2	C	280	ASN
2	C	370	ASN
2	C	450	ASN
2	C	544	ASN
2	C	641	ASN
2	C	703	ASN
2	C	901	GLN
2	C	949	GLN
2	C	965	GLN
2	C	1002	GLN
2	C	1135	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

26 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	J	1	2,3	14,14,15	0.41	0	17,19,21	2.58	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	J	2	3	14,14,15	0.38	0	17,19,21	0.69	1 (5%)
3	NAG	K	1	2,3	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	K	2	3	14,14,15	0.20	0	17,19,21	0.37	0
3	NAG	L	1	2,3	14,14,15	0.27	0	17,19,21	0.50	0
3	NAG	L	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	M	1	2,3	14,14,15	0.41	0	17,19,21	0.78	1 (5%)
3	NAG	M	2	3	14,14,15	0.42	0	17,19,21	1.23	2 (11%)
3	NAG	N	1	2,3	14,14,15	0.40	0	17,19,21	0.47	0
3	NAG	N	2	3	14,14,15	0.39	0	17,19,21	0.61	0
3	NAG	R	1	2,3	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	R	2	3	14,14,15	0.21	0	17,19,21	0.36	0
3	NAG	S	1	2,3	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	S	2	3	14,14,15	0.16	0	17,19,21	0.44	0
3	NAG	T	1	2,3	14,14,15	0.40	0	17,19,21	0.96	2 (11%)
3	NAG	T	2	3	14,14,15	0.40	0	17,19,21	1.05	2 (11%)
3	NAG	U	1	2,3	14,14,15	0.41	0	17,19,21	0.58	0
3	NAG	U	2	3	14,14,15	0.39	0	17,19,21	0.39	0
3	NAG	X	1	2,3	14,14,15	0.36	0	17,19,21	0.44	0
3	NAG	X	2	3	14,14,15	0.17	0	17,19,21	0.46	0
3	NAG	Y	1	2,3	14,14,15	0.39	0	17,19,21	0.89	1 (5%)
3	NAG	Y	2	3	14,14,15	0.38	0	17,19,21	1.27	2 (11%)
3	NAG	Z	1	2,3	14,14,15	0.41	0	17,19,21	1.13	1 (5%)
3	NAG	Z	2	3	14,14,15	0.39	0	17,19,21	0.43	0
3	NAG	a	1	2,3	14,14,15	0.39	0	17,19,21	0.37	0
3	NAG	a	2	3	14,14,15	0.23	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	1	2,3	-	5/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
3	NAG	K	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	NAG	L	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	N	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	NAG	R	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
3	NAG	U	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	X	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Y	1	2,3	-	5/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	4/6/23/26	0/1/1/1
3	NAG	Z	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	NAG	a	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1	NAG	O5-C1-C2	8.77	124.86	111.29
3	Z	1	NAG	O5-C1-C2	-4.04	105.04	111.29
3	Y	2	NAG	O5-C1-C2	3.99	117.46	111.29
3	J	1	NAG	C1-O5-C5	3.85	117.35	112.19
3	M	2	NAG	C1-O5-C5	3.42	116.77	112.19
3	Y	2	NAG	C1-O5-C5	2.88	116.04	112.19
3	Y	1	NAG	C1-O5-C5	2.71	115.81	112.19
3	M	2	NAG	O5-C1-C2	2.65	115.39	111.29
3	T	2	NAG	O5-C1-C2	2.64	115.37	111.29
3	T	1	NAG	O5-C1-C2	2.62	115.35	111.29
3	T	2	NAG	C1-C2-N2	2.48	114.34	110.43
3	J	1	NAG	C1-C2-N2	2.39	114.19	110.43
3	J	1	NAG	C4-C3-C2	-2.29	107.66	111.02
3	J	2	NAG	C1-O5-C5	2.26	115.22	112.19
3	T	1	NAG	C1-C2-N2	2.15	113.82	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	1	NAG	C2-N2-C7	-2.07	120.12	122.90
3	J	1	NAG	C3-C4-C5	-2.04	106.54	110.23

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	1	NAG	C1-C2-N2-C7
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C1-C2-N2-C7
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C1-C2-N2-C7
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	Y	1	NAG	C1-C2-N2-C7
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
3	J	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
3	U	2	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	Z	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O7-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
3	a	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	Y	2	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	N	1	NAG	C8-C7-N2-C2
3	a	1	NAG	C4-C5-C6-O6
3	N	2	NAG	C8-C7-N2-C2
3	L	1	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	X	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O7-C7-N2-C2
3	N	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6

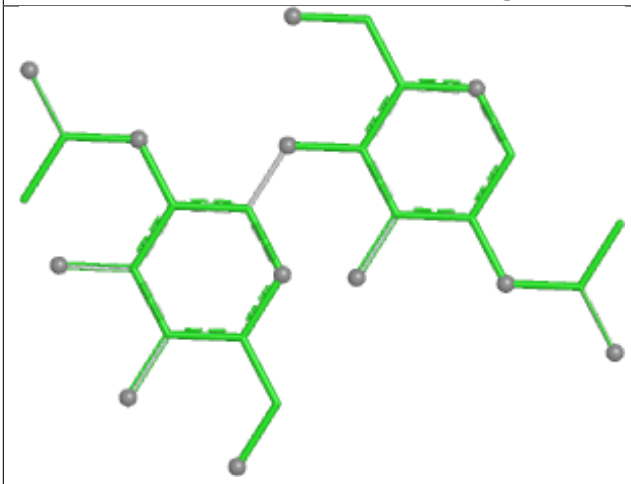
There are no ring outliers.

2 monomers are involved in 3 short contacts:

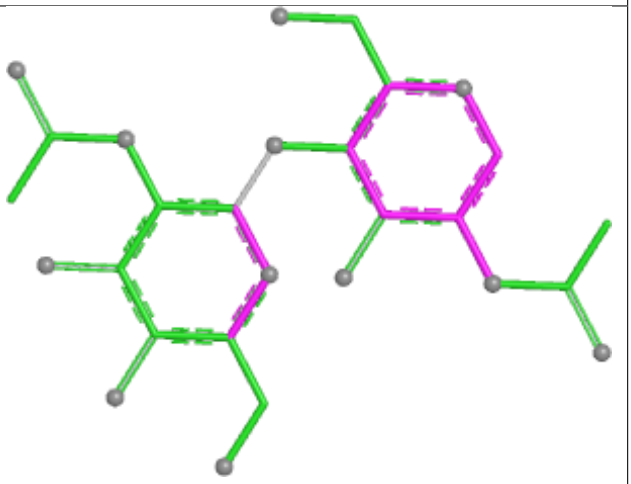
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	NAG	2	0
3	R	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

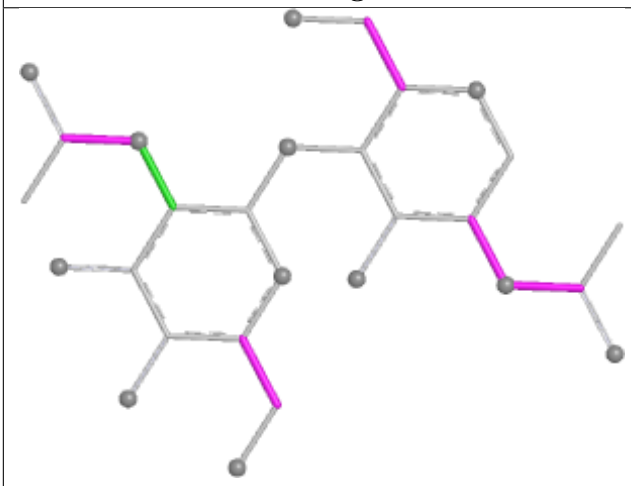
Oligosaccharide Chain J



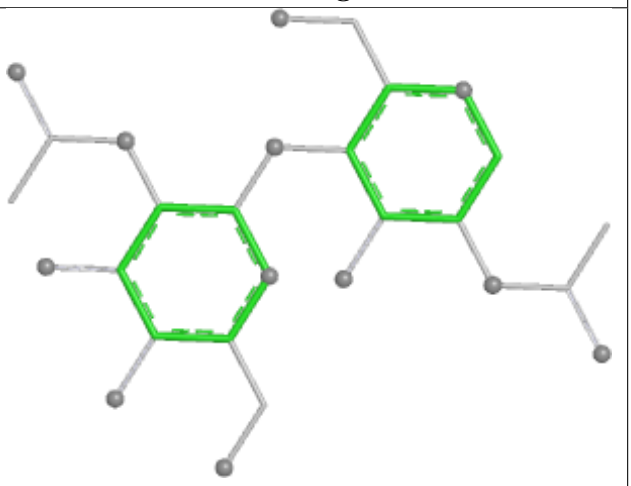
Bond lengths



Bond angles

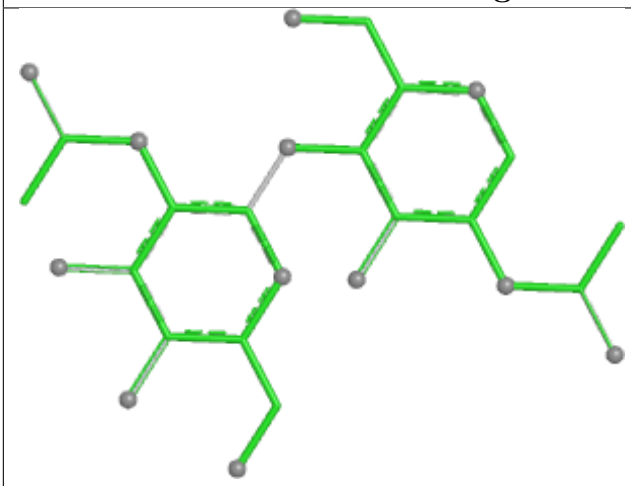


Torsions

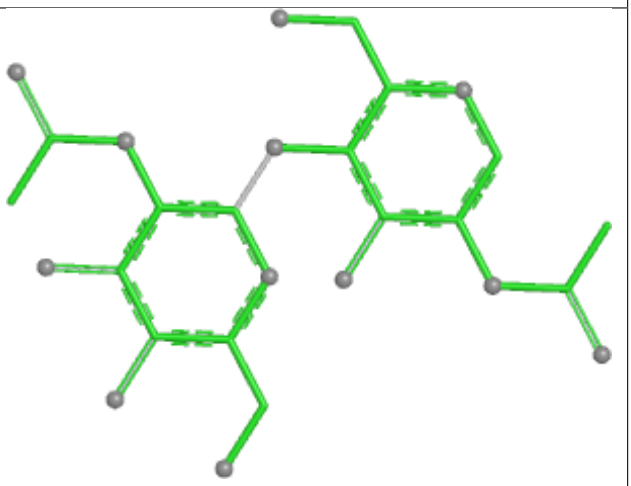


Rings

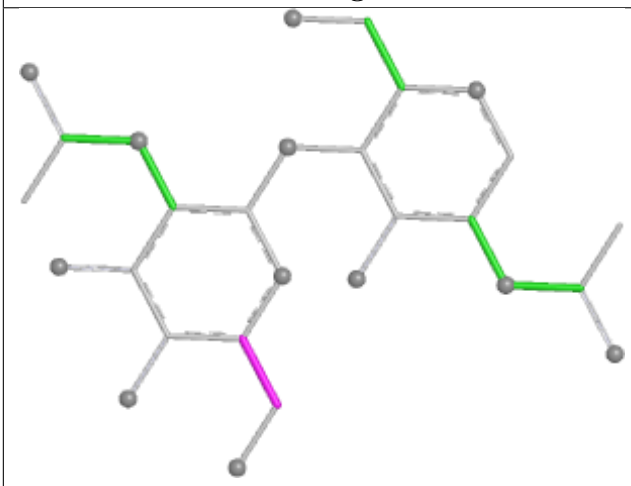
Oligosaccharide Chain K



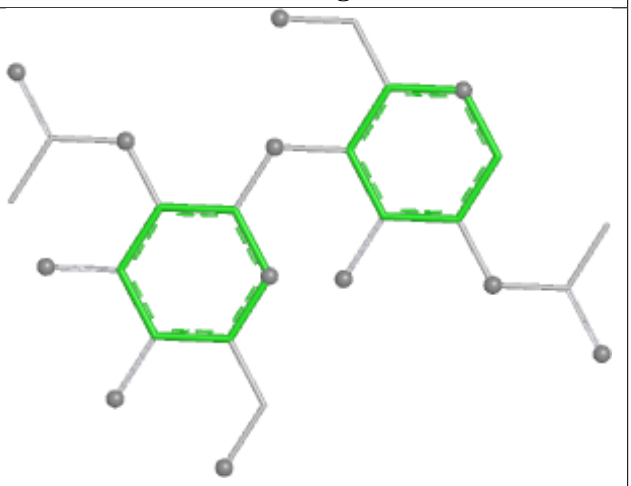
Bond lengths



Bond angles

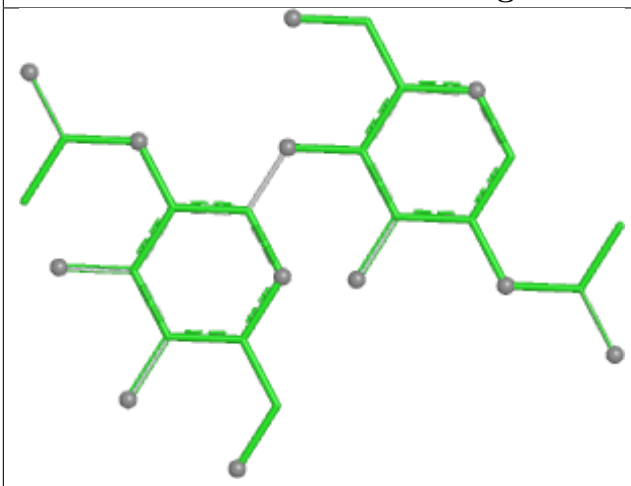


Torsions

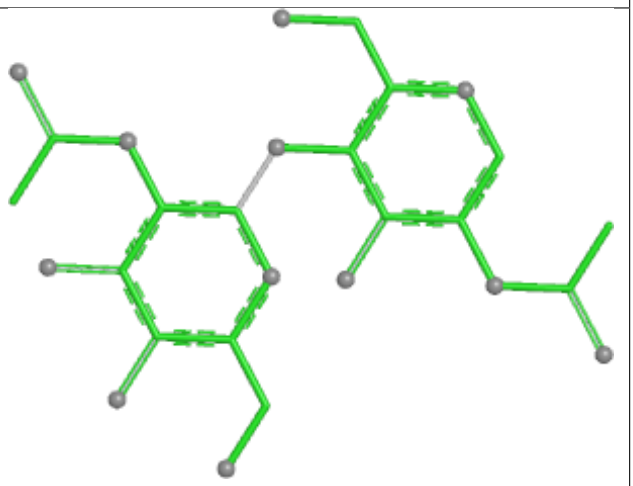


Rings

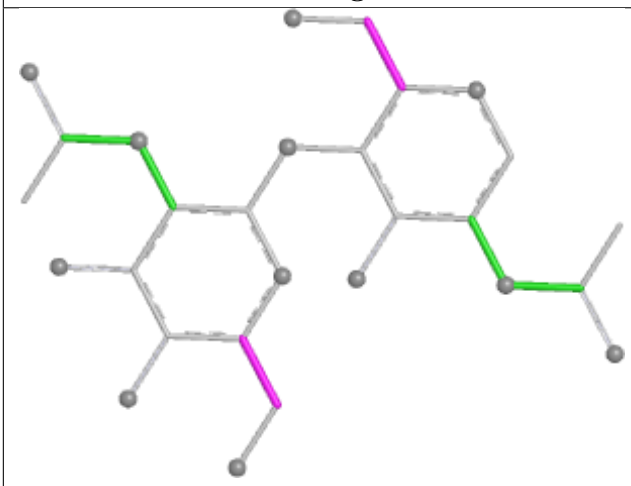
Oligosaccharide Chain L



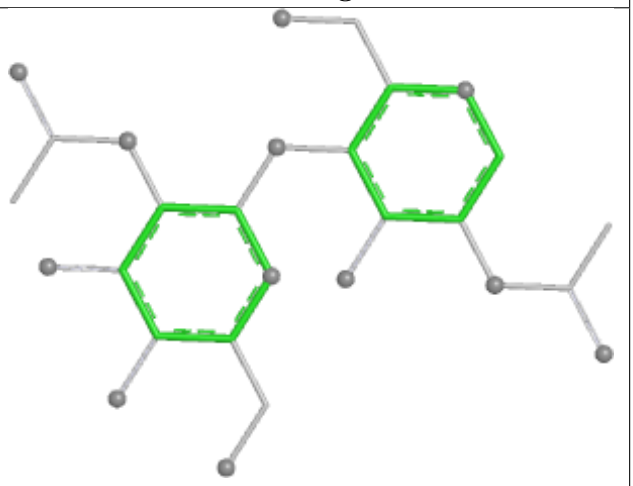
Bond lengths



Bond angles

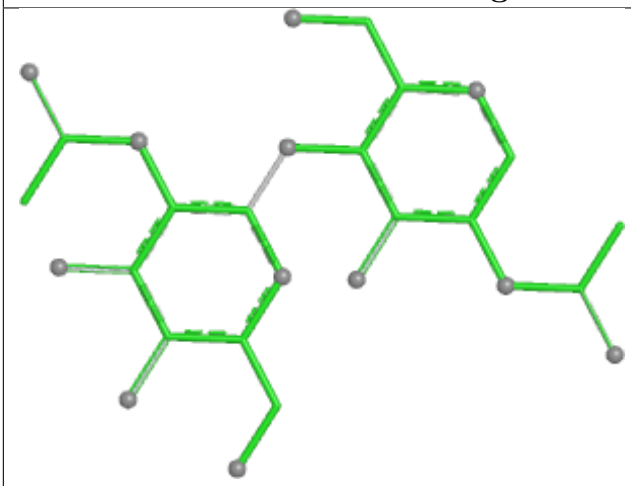


Torsions

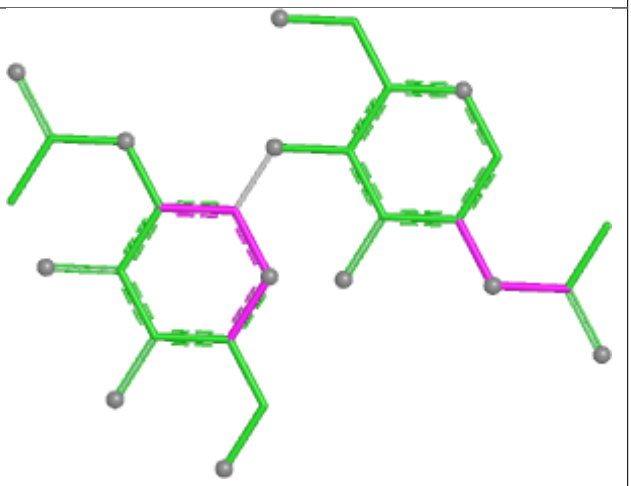


Rings

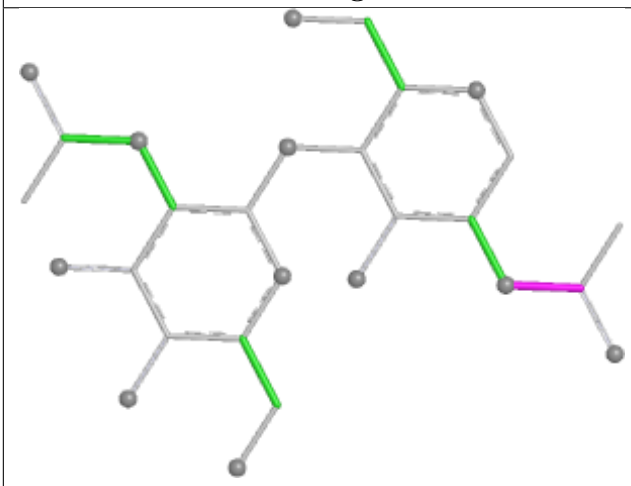
Oligosaccharide Chain M



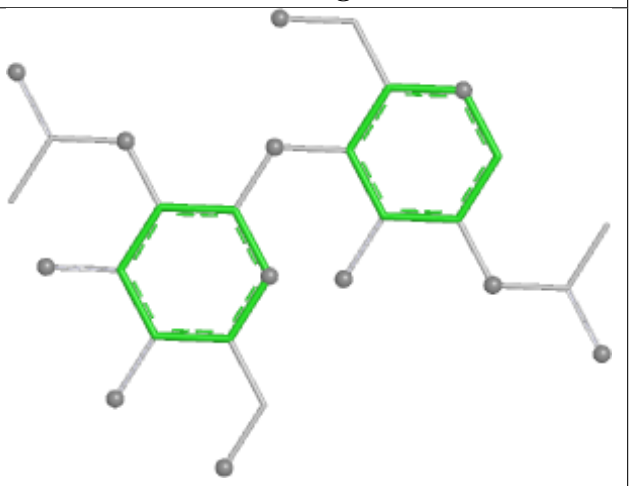
Bond lengths



Bond angles

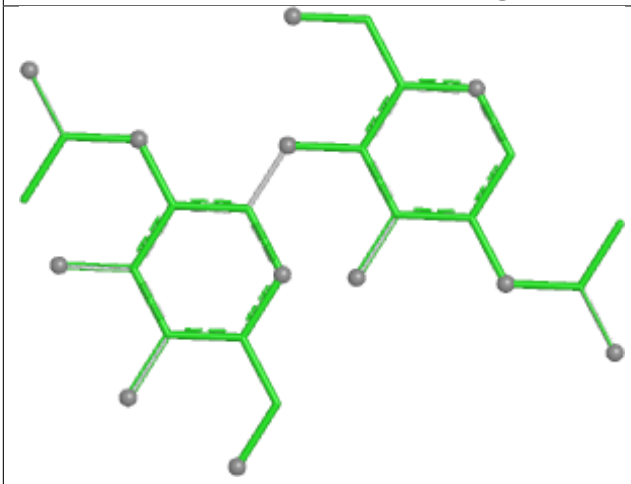


Torsions

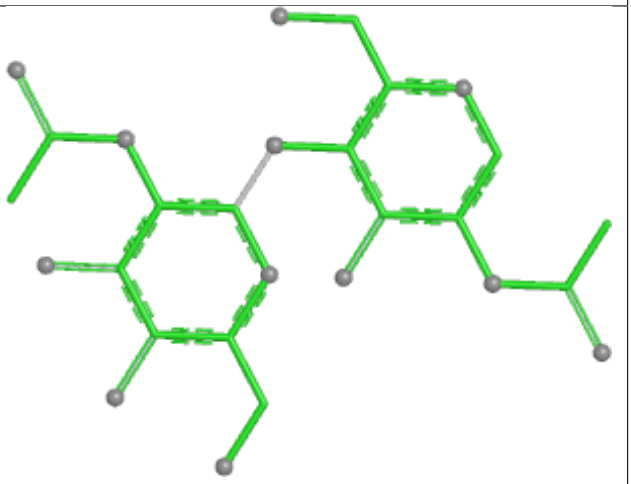


Rings

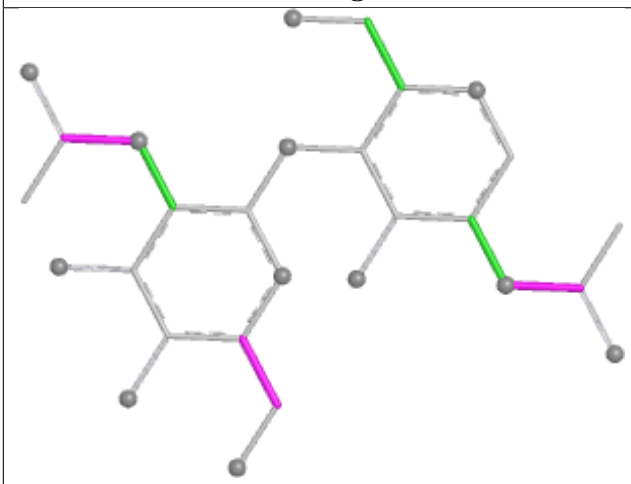
Oligosaccharide Chain N



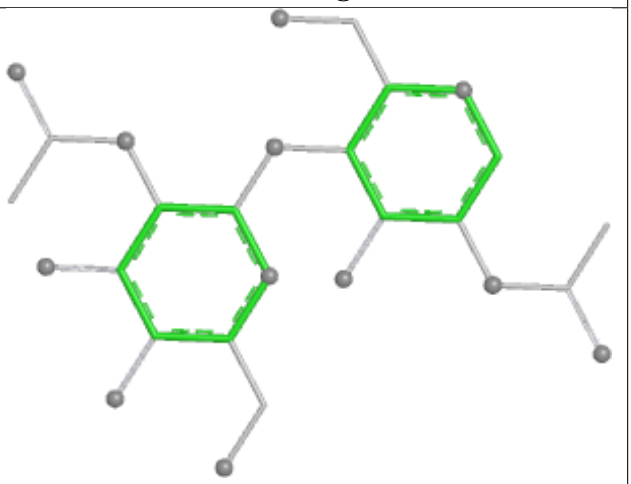
Bond lengths



Bond angles

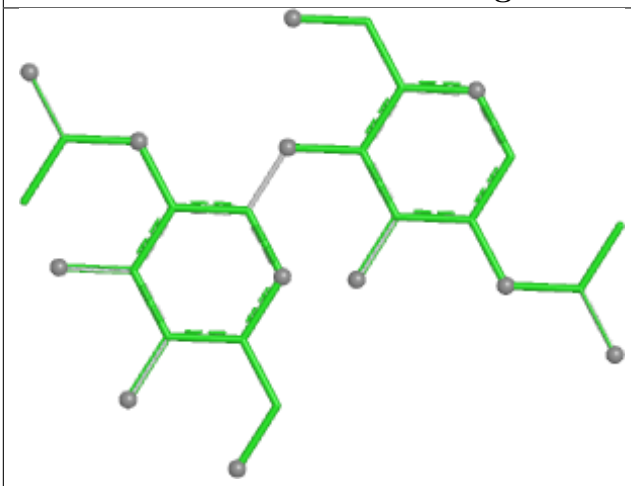


Torsions

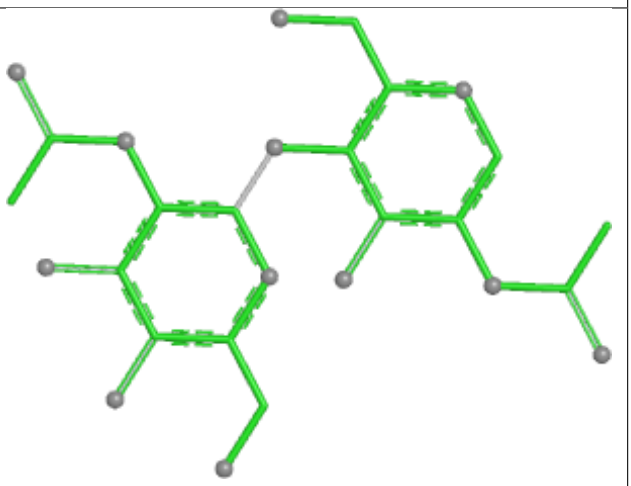


Rings

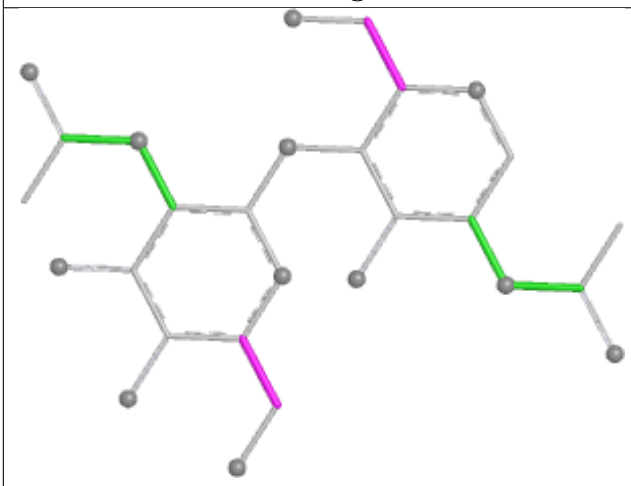
Oligosaccharide Chain R



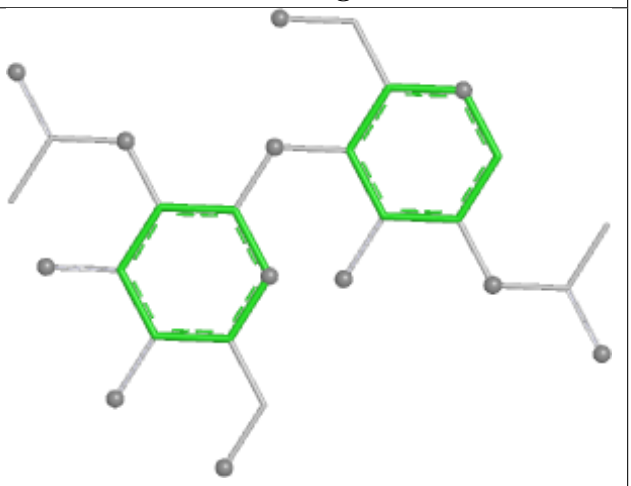
Bond lengths



Bond angles

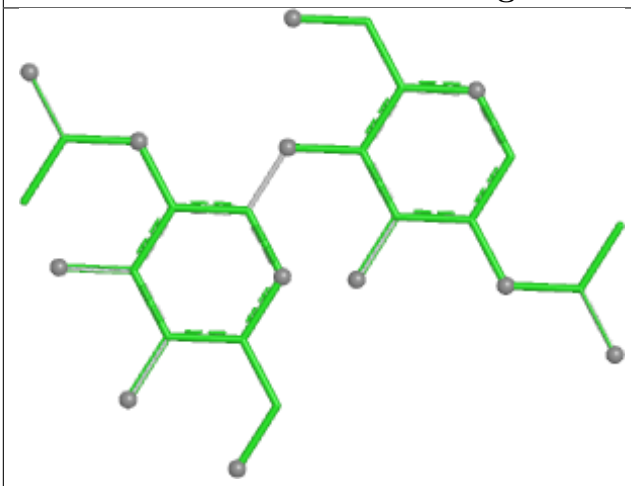


Torsions

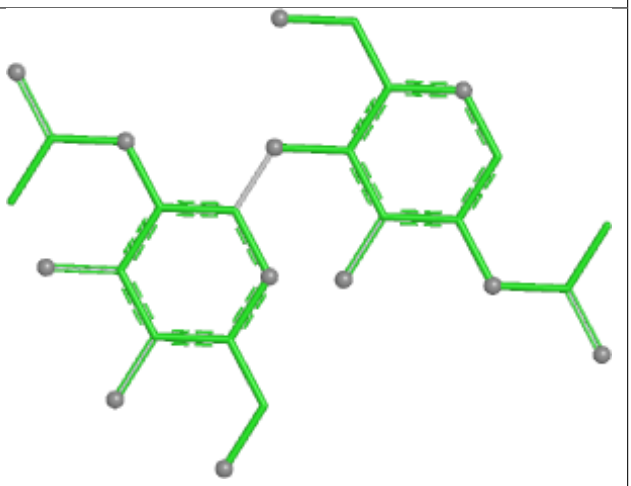


Rings

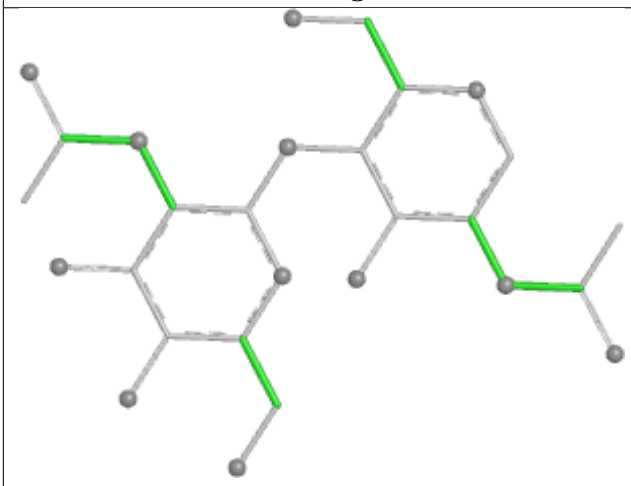
Oligosaccharide Chain S



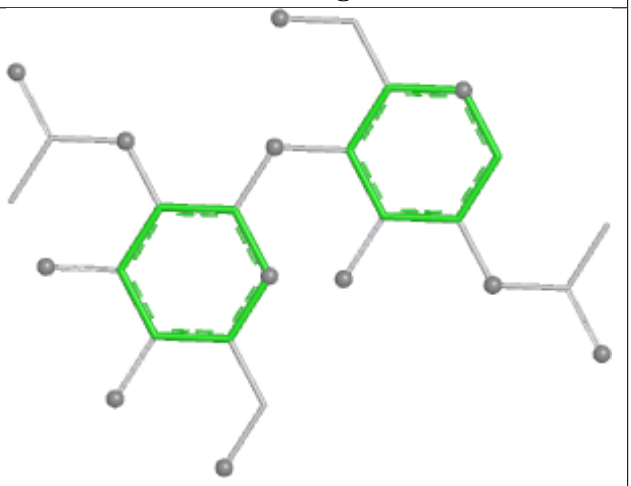
Bond lengths



Bond angles

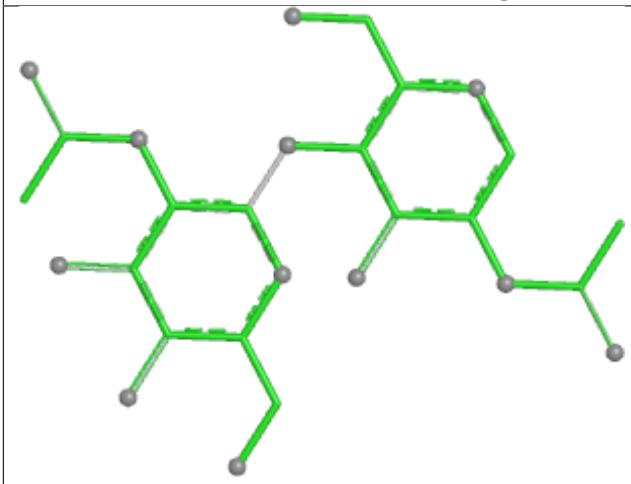


Torsions

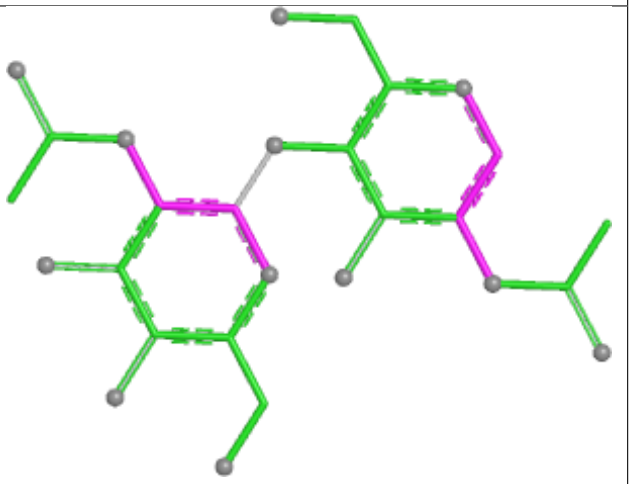


Rings

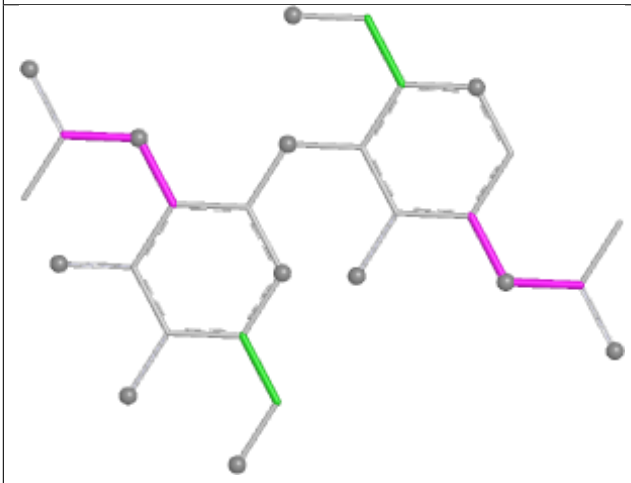
Oligosaccharide Chain T



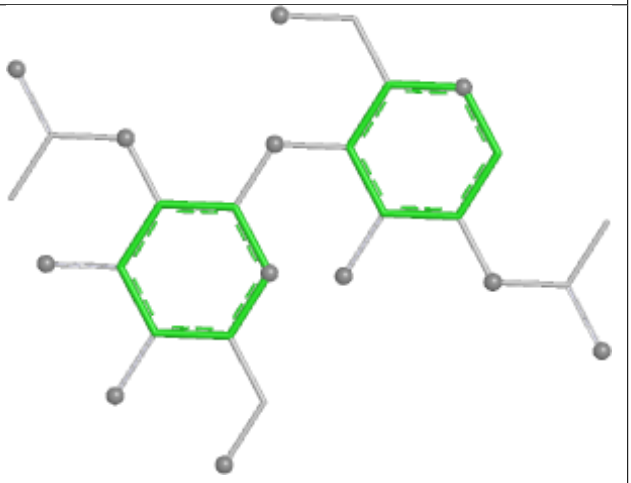
Bond lengths



Bond angles

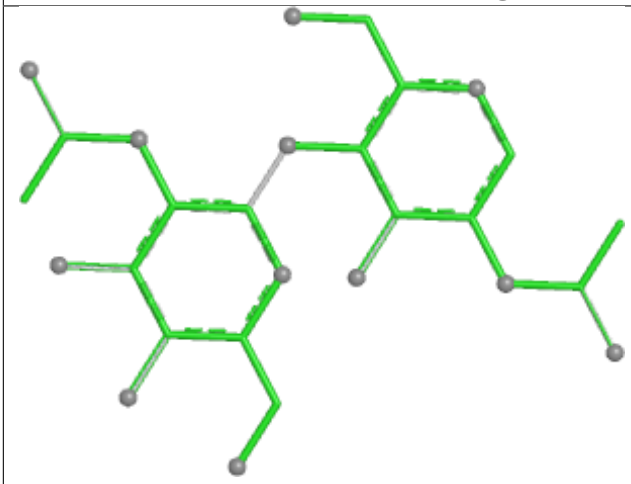


Torsions

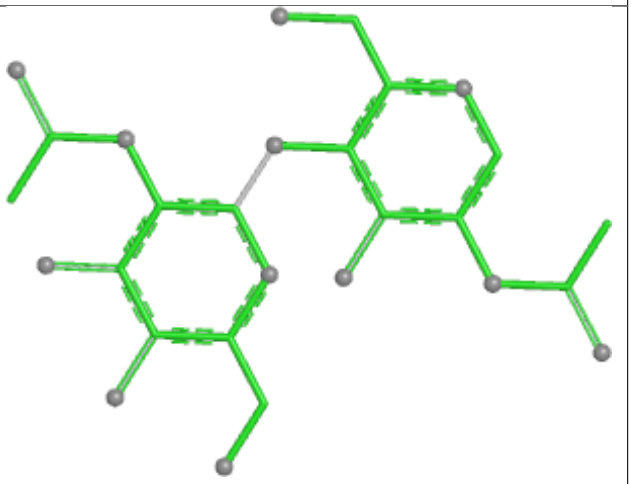


Rings

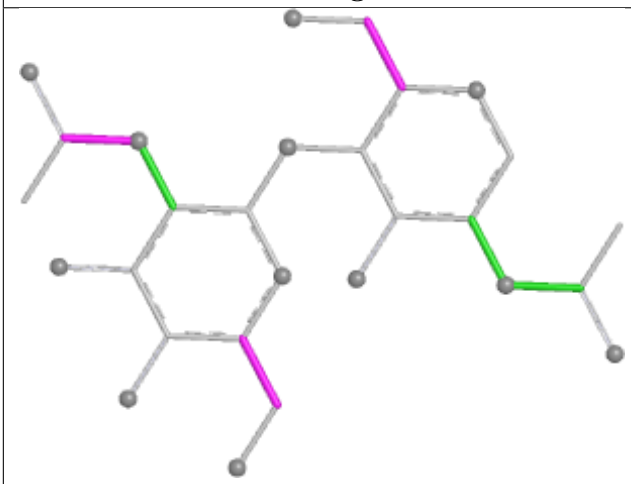
Oligosaccharide Chain U



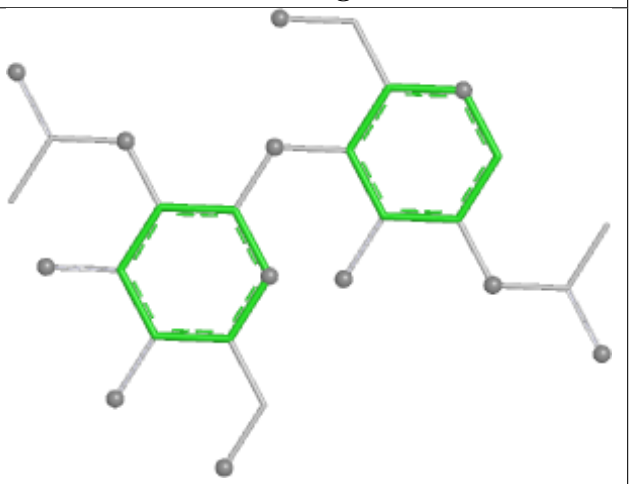
Bond lengths



Bond angles

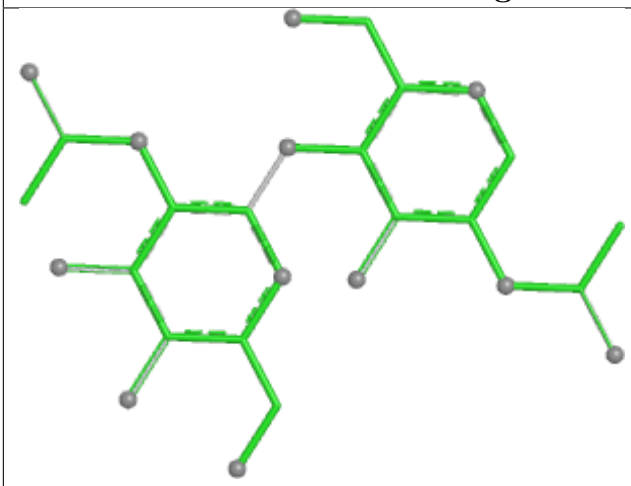


Torsions

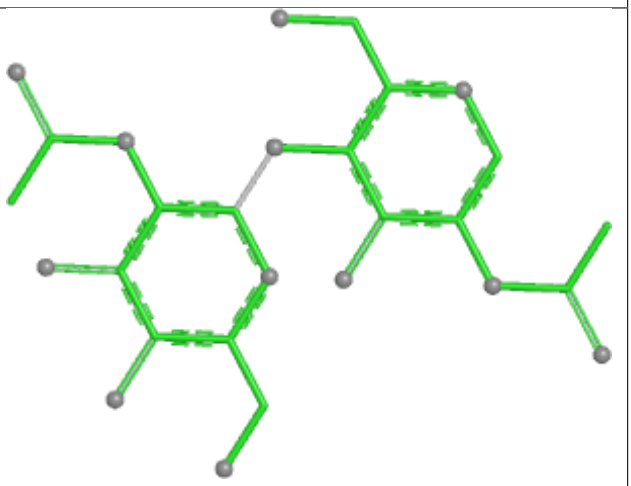


Rings

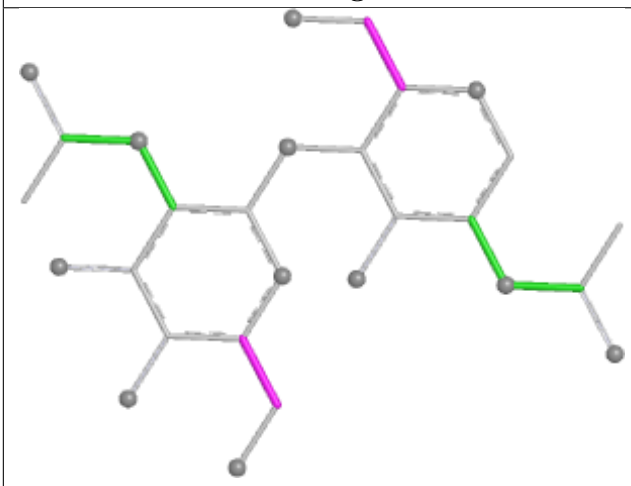
Oligosaccharide Chain X



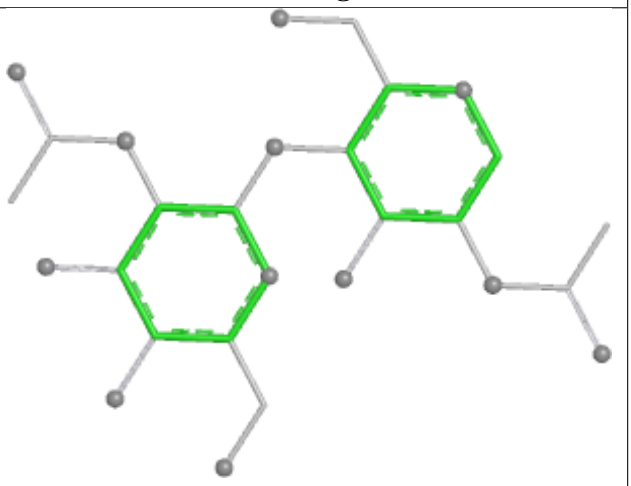
Bond lengths



Bond angles

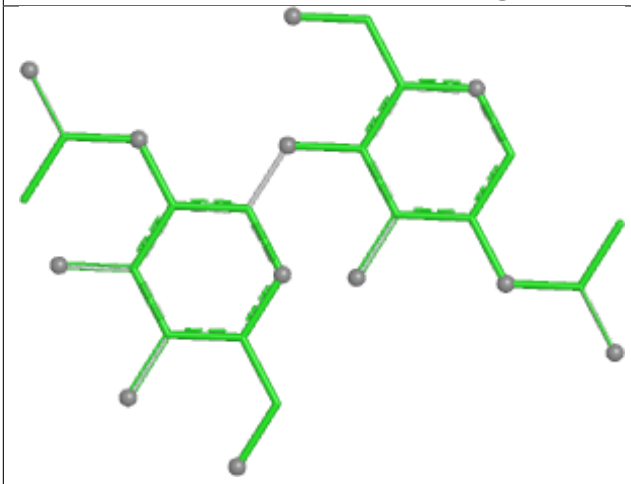


Torsions

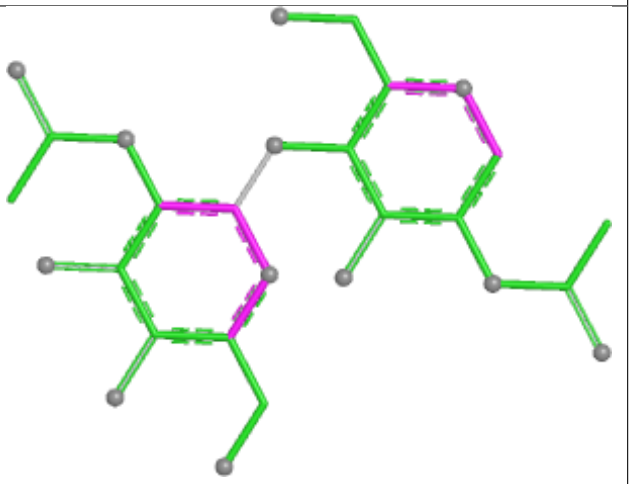


Rings

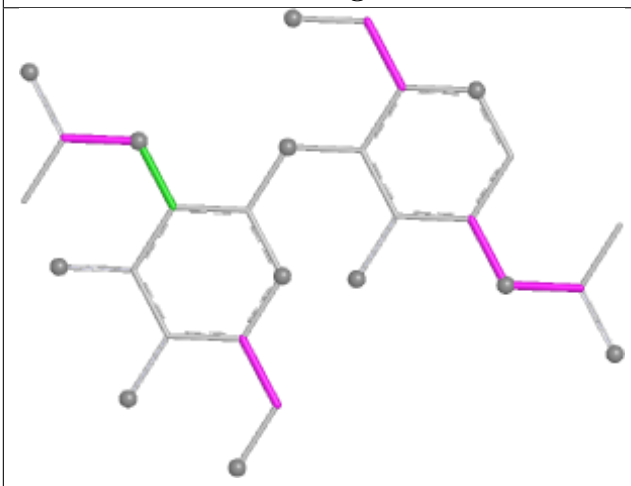
Oligosaccharide Chain Y



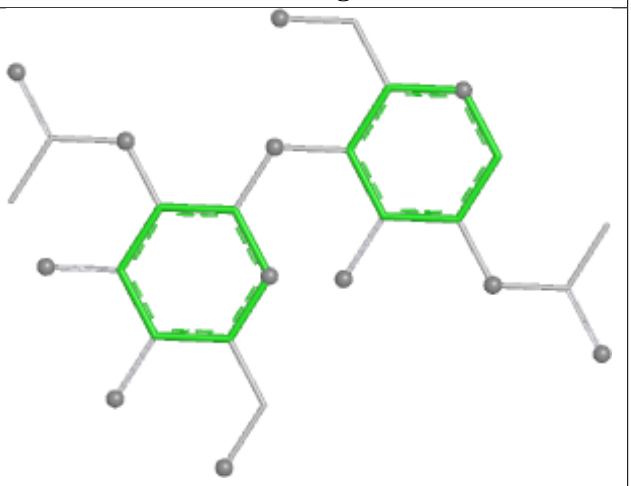
Bond lengths



Bond angles

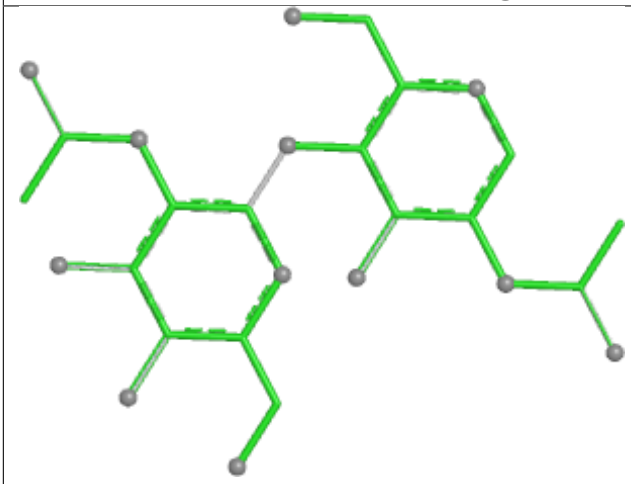


Torsions

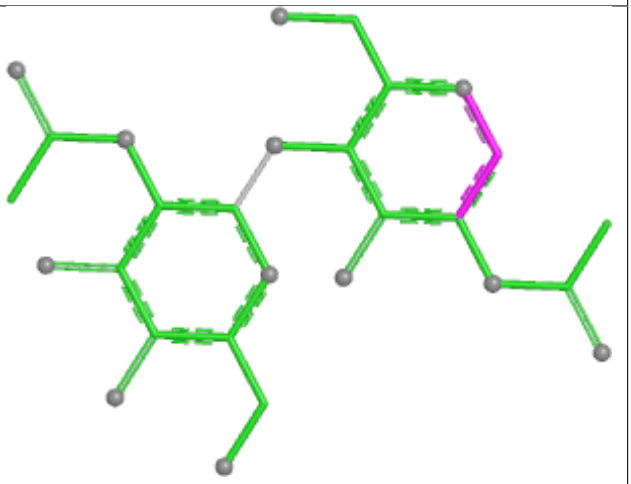


Rings

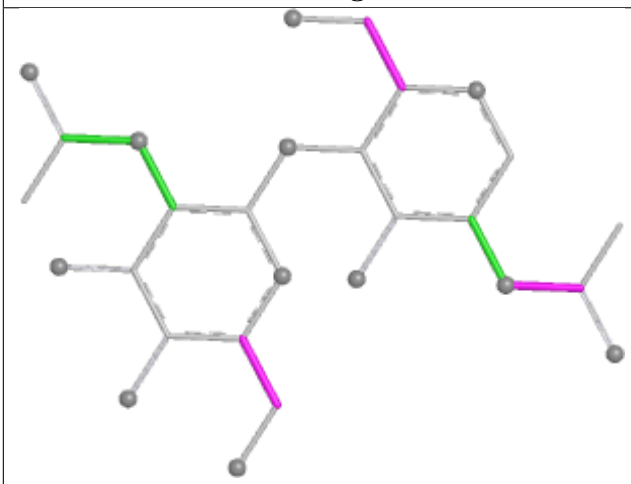
Oligosaccharide Chain Z



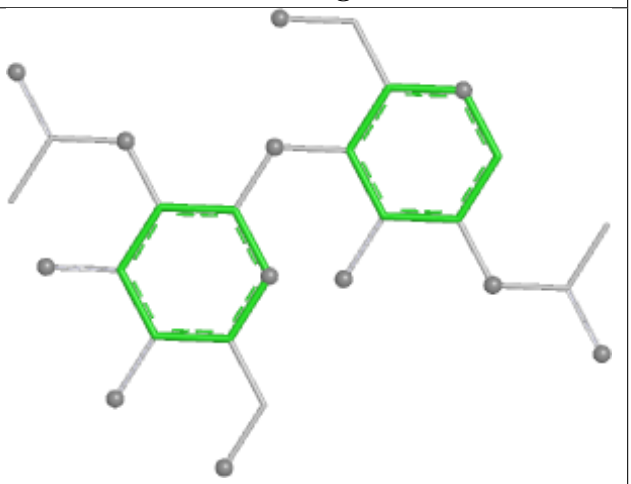
Bond lengths



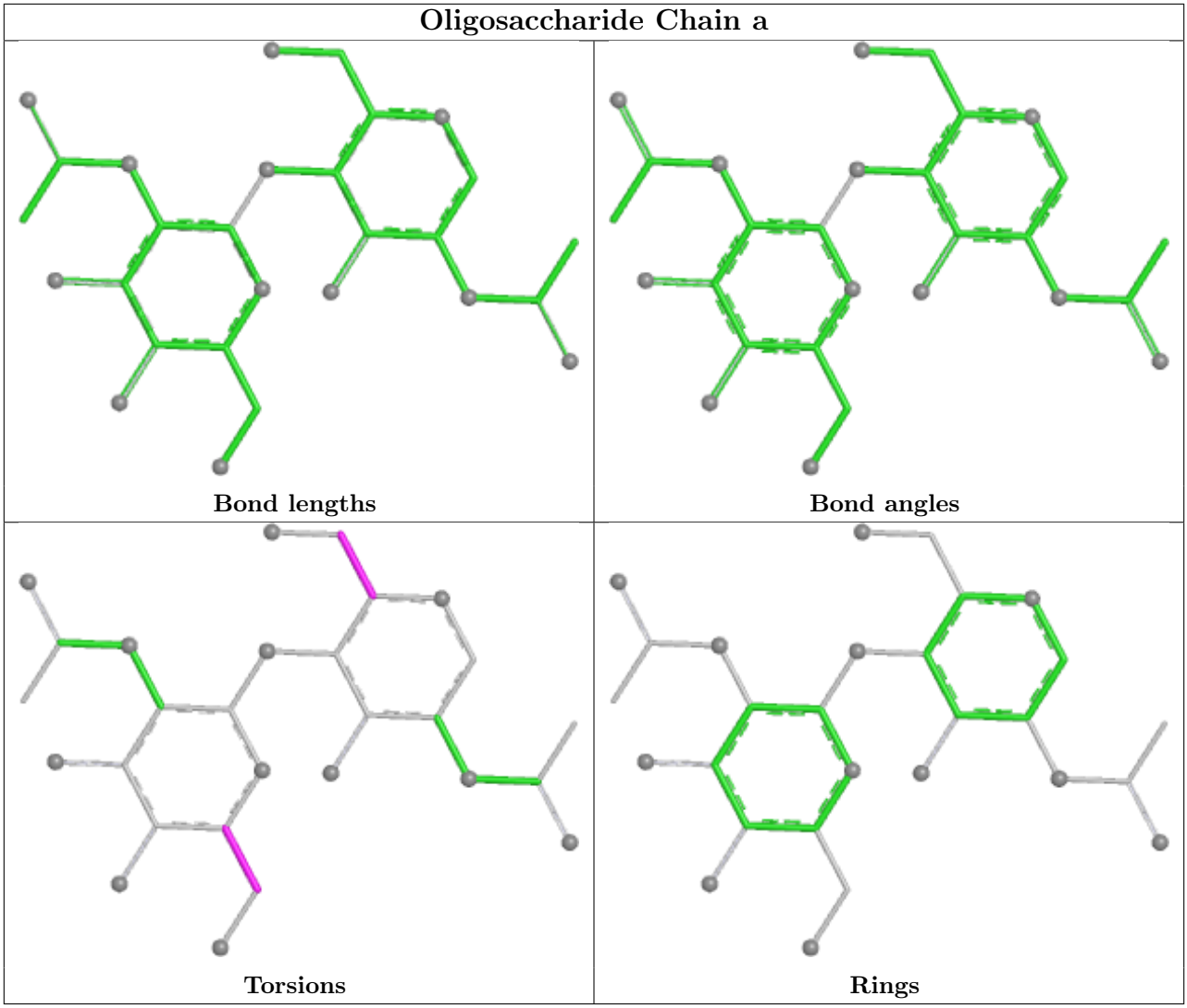
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1307	2	14,14,15	0.44	0	17,19,21	1.61	1 (5%)
4	NAG	C	1301	2	14,14,15	0.38	0	17,19,21	0.46	0
4	NAG	B	1308	2	14,14,15	0.41	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1304	2	14,14,15	0.40	0	17,19,21	0.49	0
4	NAG	A	1301	2	14,14,15	0.39	0	17,19,21	0.38	0
4	NAG	A	1306	2	14,14,15	0.38	0	17,19,21	0.35	0
4	NAG	A	1302	2	14,14,15	0.40	0	17,19,21	0.61	0
4	NAG	A	1305	2	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	A	1307	2	14,14,15	0.39	0	17,19,21	0.75	1 (5%)
4	NAG	B	1305	2	14,14,15	0.41	0	17,19,21	0.61	0
4	NAG	B	1306	-	14,14,15	0.43	0	17,19,21	0.78	1 (5%)
4	NAG	B	1302	2	14,14,15	0.39	0	17,19,21	0.76	1 (5%)
4	NAG	B	1304	2	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	A	1303	2	14,14,15	0.40	0	17,19,21	0.38	0
4	NAG	B	1303	2	14,14,15	0.39	0	17,19,21	0.36	0
4	NAG	C	1306	2	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
4	NAG	C	1304	2	14,14,15	0.40	0	17,19,21	0.41	0
4	NAG	C	1305	2	14,14,15	0.40	0	17,19,21	0.58	0
4	NAG	B	1301	2	14,14,15	0.40	0	17,19,21	0.44	0
4	NAG	C	1302	2	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	A	1308	2	14,14,15	0.42	0	17,19,21	0.88	1 (5%)
4	NAG	C	1303	2	14,14,15	0.41	0	17,19,21	0.42	0
4	NAG	C	1307	2	14,14,15	0.45	0	17,19,21	1.19	1 (5%)
4	NAG	C	1308	-	14,14,15	0.18	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1307	2	-	5/6/23/26	0/1/1/1
4	NAG	C	1301	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1308	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1304	2	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	2	-	5/6/23/26	0/1/1/1
4	NAG	A	1302	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	2	-	5/6/23/26	0/1/1/1
4	NAG	B	1305	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1302	2	-	5/6/23/26	0/1/1/1
4	NAG	B	1304	2	-	3/6/23/26	0/1/1/1
4	NAG	A	1303	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	2	-	3/6/23/26	0/1/1/1
4	NAG	C	1304	2	-	4/6/23/26	0/1/1/1
4	NAG	C	1305	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	2	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1307	NAG	O5-C1-C2	6.20	120.88	111.29
4	C	1307	NAG	O5-C1-C2	3.82	117.20	111.29
4	C	1306	NAG	C1-O5-C5	2.75	115.88	112.19
4	A	1308	NAG	O5-C1-C2	2.64	115.38	111.29
4	B	1306	NAG	O5-C1-C2	2.31	114.87	111.29
4	B	1302	NAG	O5-C1-C2	-2.08	108.08	111.29
4	A	1307	NAG	O5-C1-C2	2.02	114.42	111.29

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	A	1303	NAG	O7-C7-N2-C2
4	A	1306	NAG	C1-C2-N2-C7
4	A	1306	NAG	C8-C7-N2-C2
4	A	1306	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1304	NAG	C3-C2-N2-C7
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	B	1307	NAG	C1-C2-N2-C7
4	B	1307	NAG	C8-C7-N2-C2
4	B	1307	NAG	O7-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1306	NAG	C1-C2-N2-C7
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	C	1307	NAG	C8-C7-N2-C2
4	C	1307	NAG	O7-C7-N2-C2
4	A	1303	NAG	C8-C7-N2-C2
4	A	1307	NAG	C8-C7-N2-C2
4	A	1307	NAG	O7-C7-N2-C2
4	B	1306	NAG	C8-C7-N2-C2
4	B	1306	NAG	O7-C7-N2-C2
4	C	1304	NAG	O5-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	B	1303	NAG	C8-C7-N2-C2
4	C	1301	NAG	C8-C7-N2-C2
4	A	1306	NAG	O5-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	A	1307	NAG	O5-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	C	1301	NAG	O7-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	C	1305	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1305	NAG	C8-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	A	1304	NAG	C1-C2-N2-C7
4	A	1307	NAG	C1-C2-N2-C7
4	B	1302	NAG	C1-C2-N2-C7
4	B	1302	NAG	O5-C5-C6-O6
4	B	1306	NAG	C3-C2-N2-C7
4	B	1308	NAG	O7-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	NAG	1	0
4	A	1307	NAG	1	0
4	B	1302	NAG	1	0
4	C	1306	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

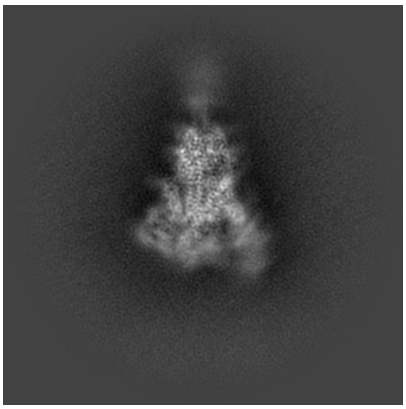
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36879. These allow visual inspection of the internal detail of the map and identification of artifacts.

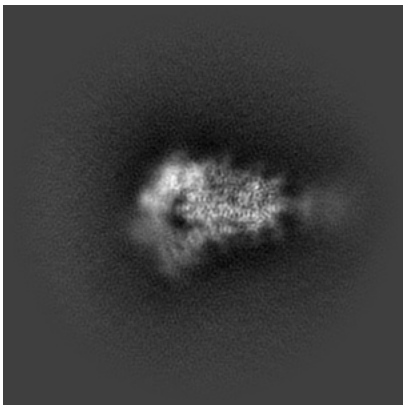
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

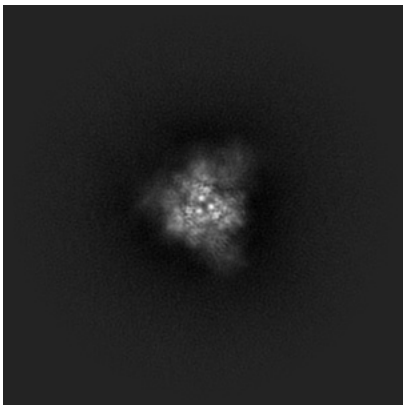
6.1.1 Primary map



X

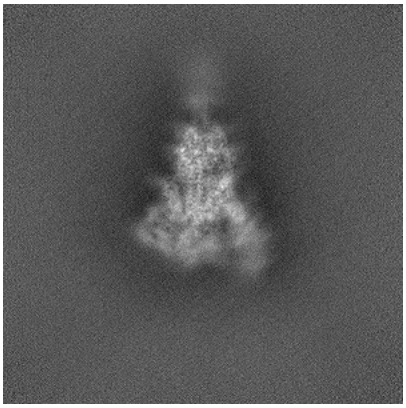


Y

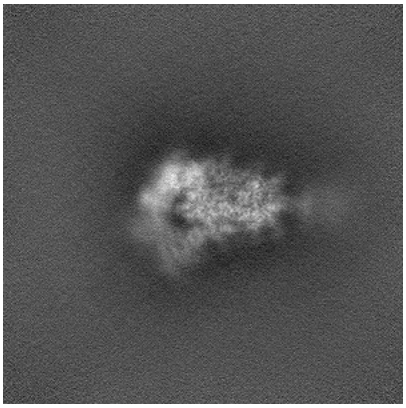


Z

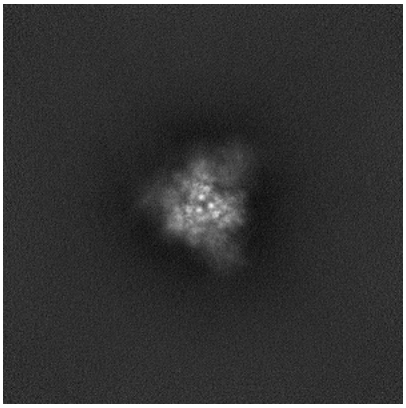
6.1.2 Raw map



X



Y

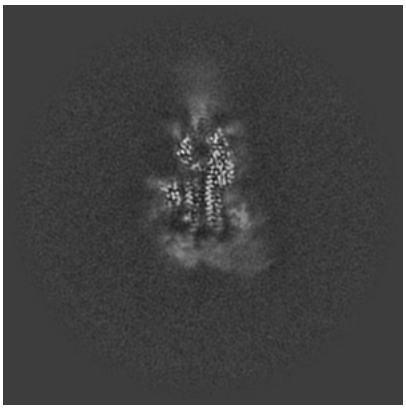


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

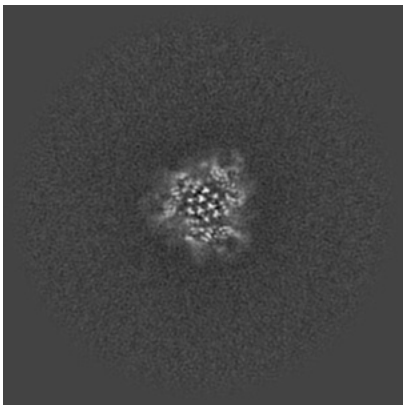
6.2.1 Primary map



X Index: 256

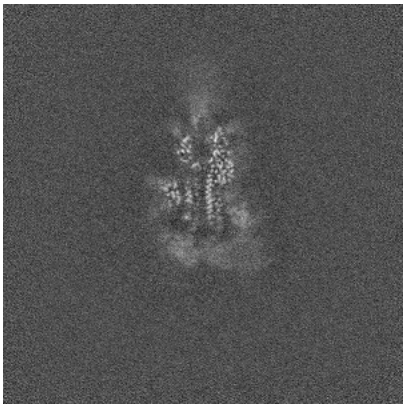


Y Index: 256



Z Index: 256

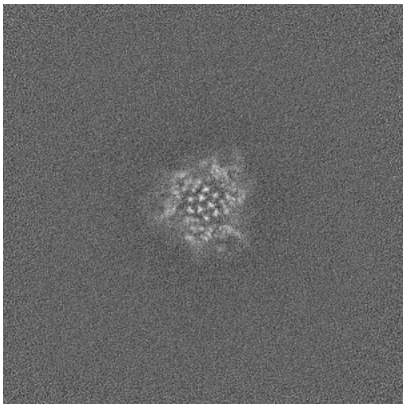
6.2.2 Raw map



X Index: 256



Y Index: 256

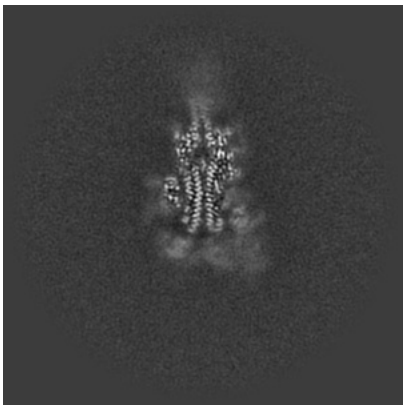


Z Index: 256

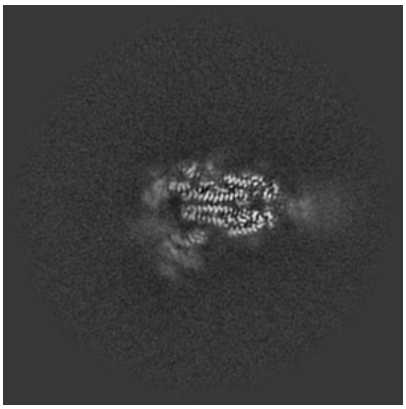
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

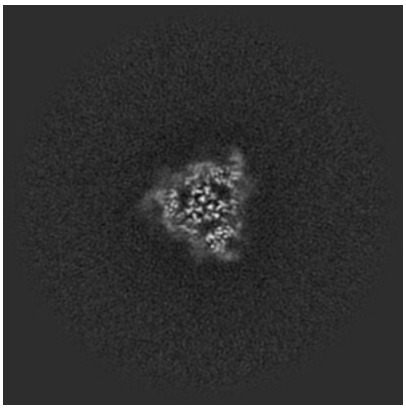
6.3.1 Primary map



X Index: 252

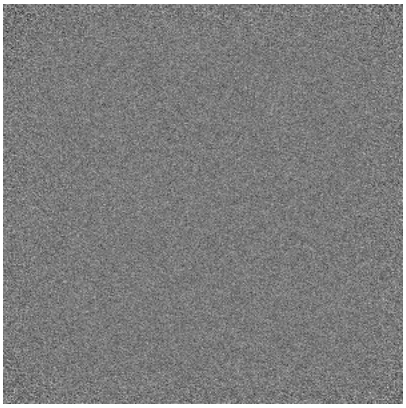


Y Index: 251

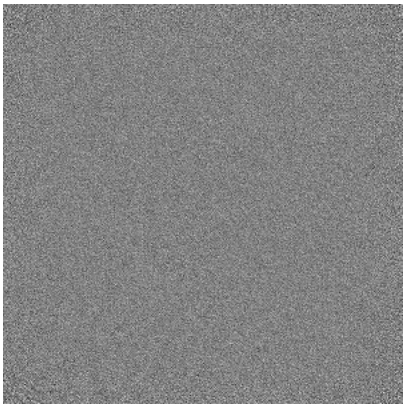


Z Index: 251

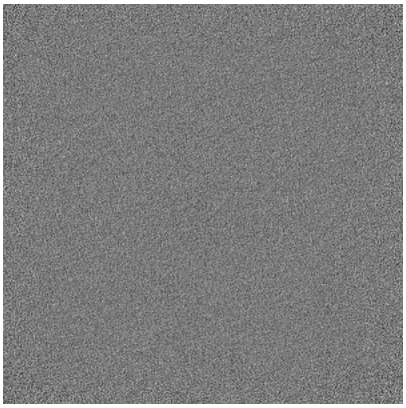
6.3.2 Raw map



X Index: 0



Y Index: 0

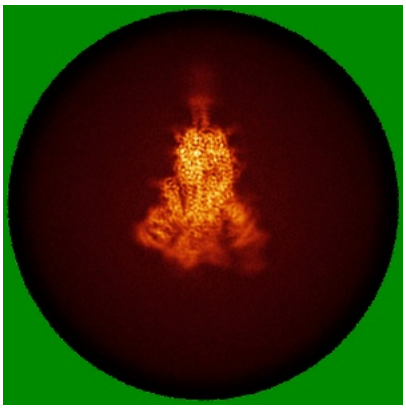


Z Index: 0

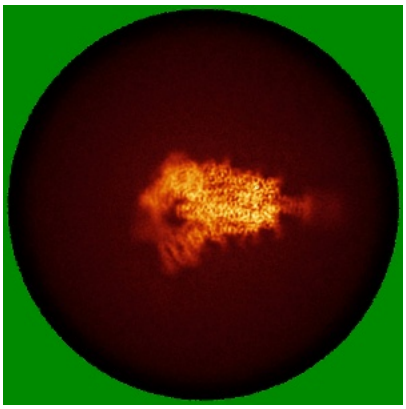
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

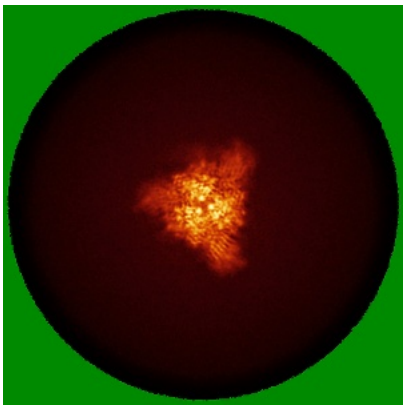
6.4.1 Primary map



X

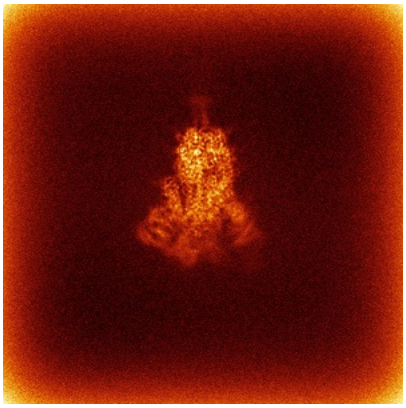


Y

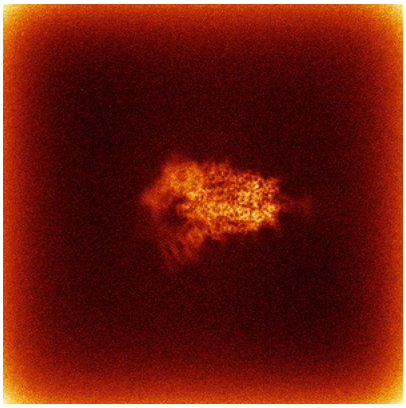


Z

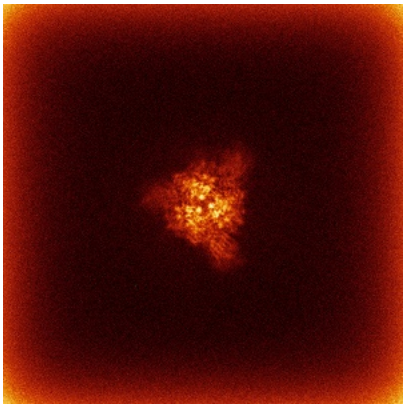
6.4.2 Raw map



X



Y

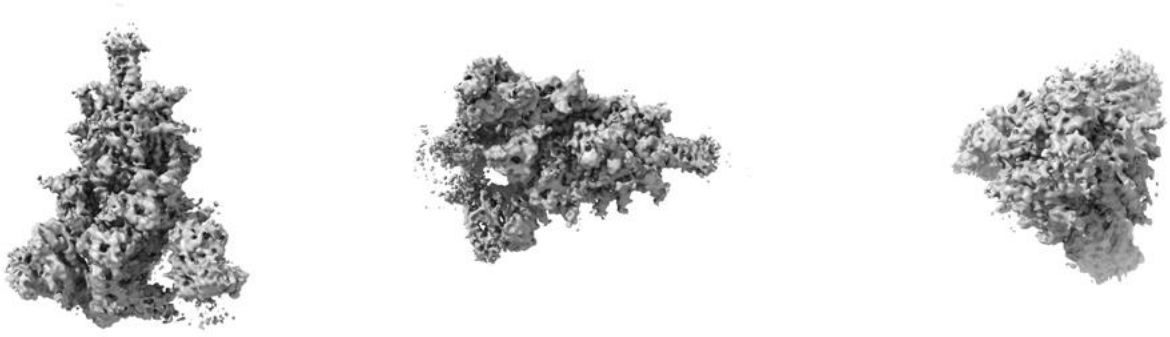


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

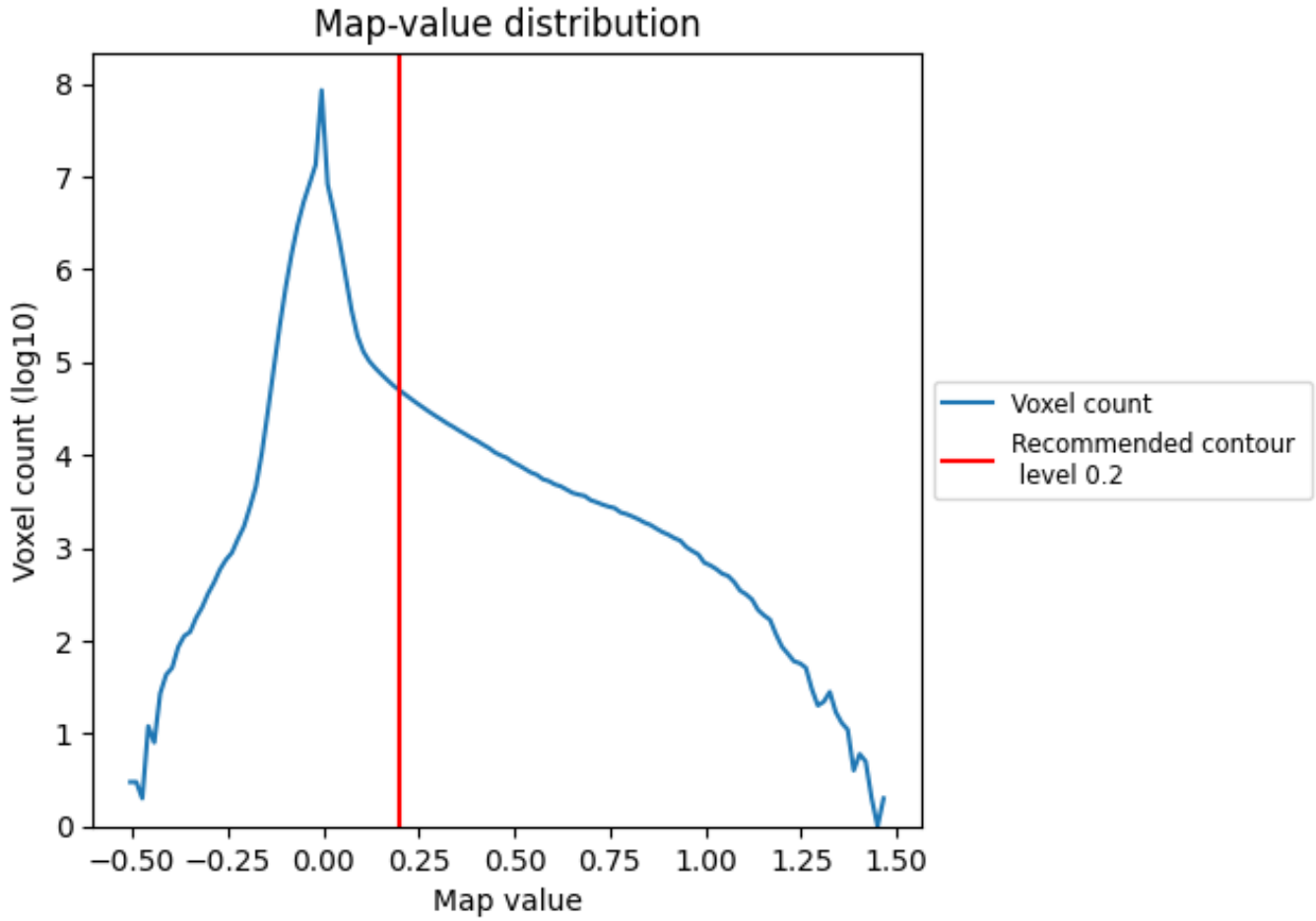
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

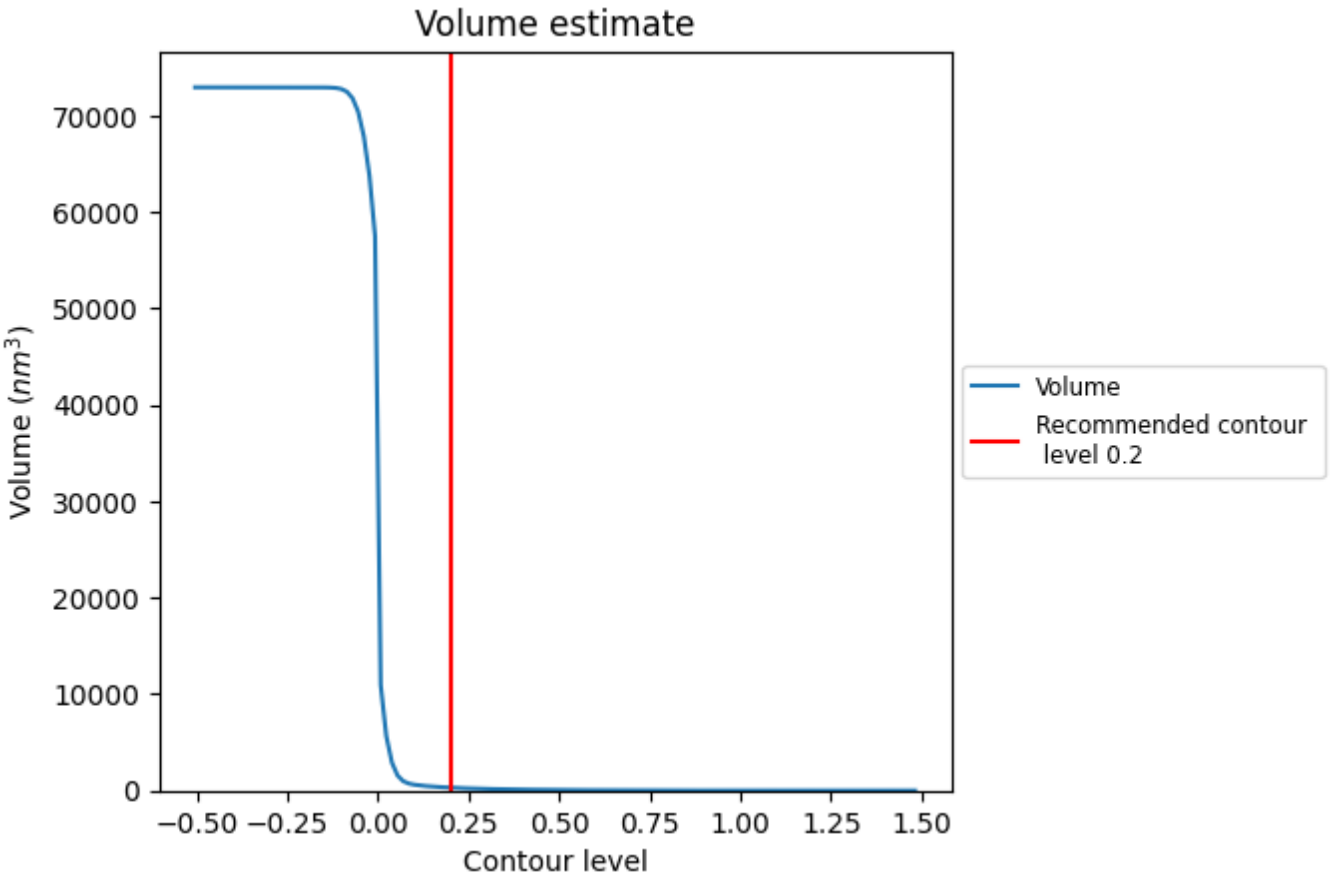
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

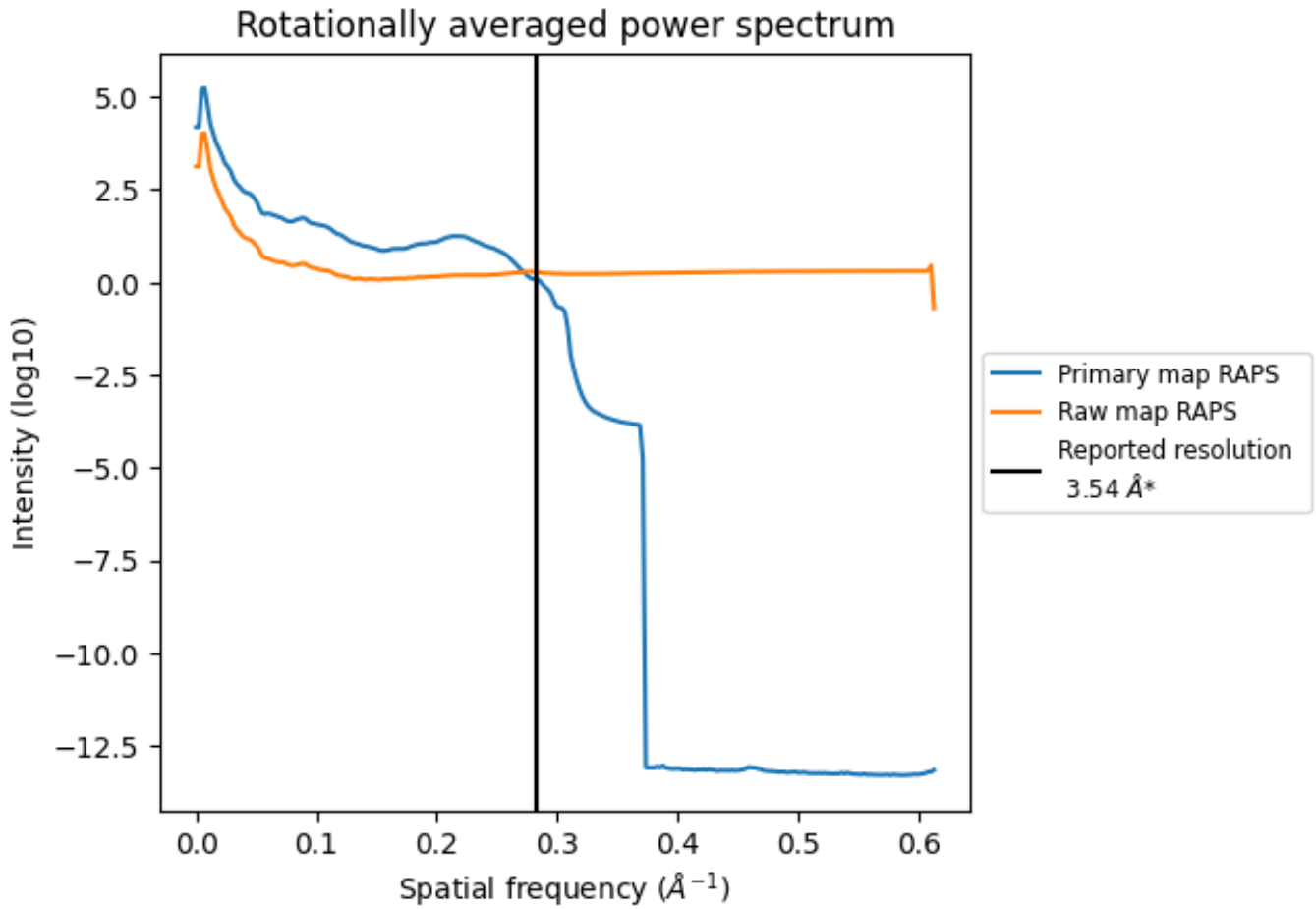
7.2 Volume estimate



The volume at the recommended contour level is 302 nm^3; this corresponds to an approximate mass of 273 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

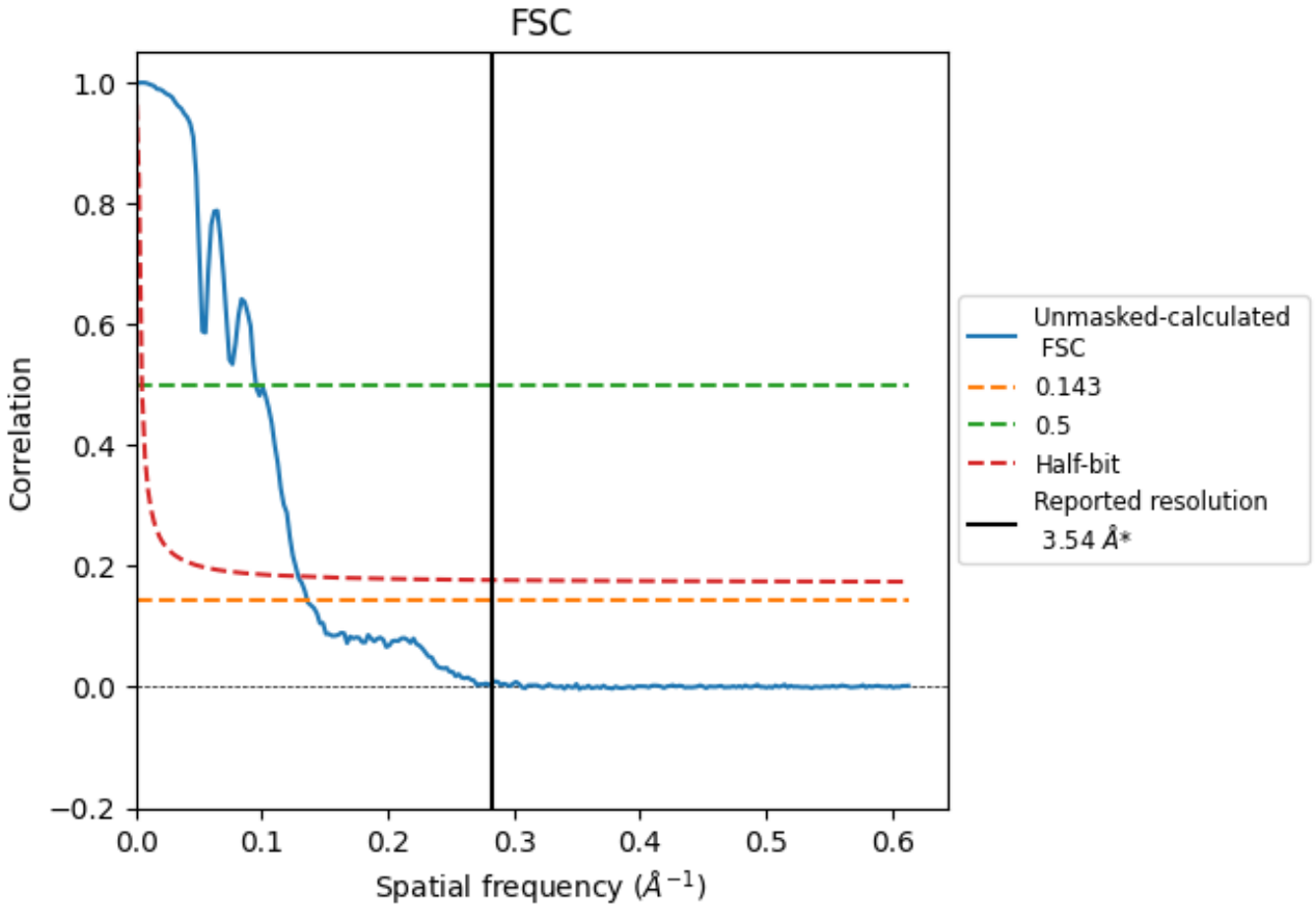


*Reported resolution corresponds to spatial frequency of 0.282 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

8.2 Resolution estimates (i)

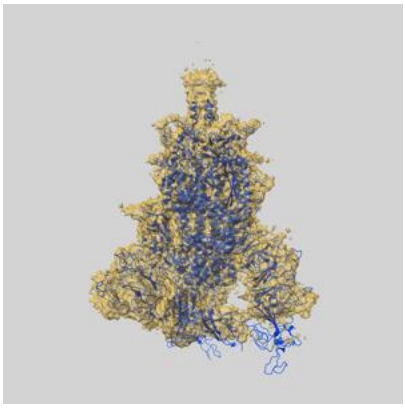
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.35	10.49	7.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.35 differs from the reported value 3.54 by more than 10 %

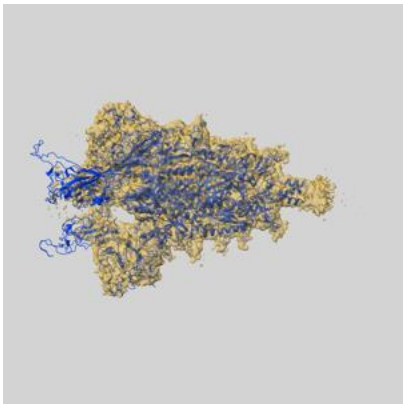
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36879 and PDB model 8K47. Per-residue inclusion information can be found in section 3 on page 16.

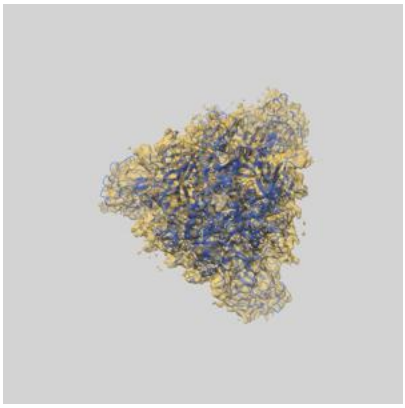
9.1 Map-model overlay



X



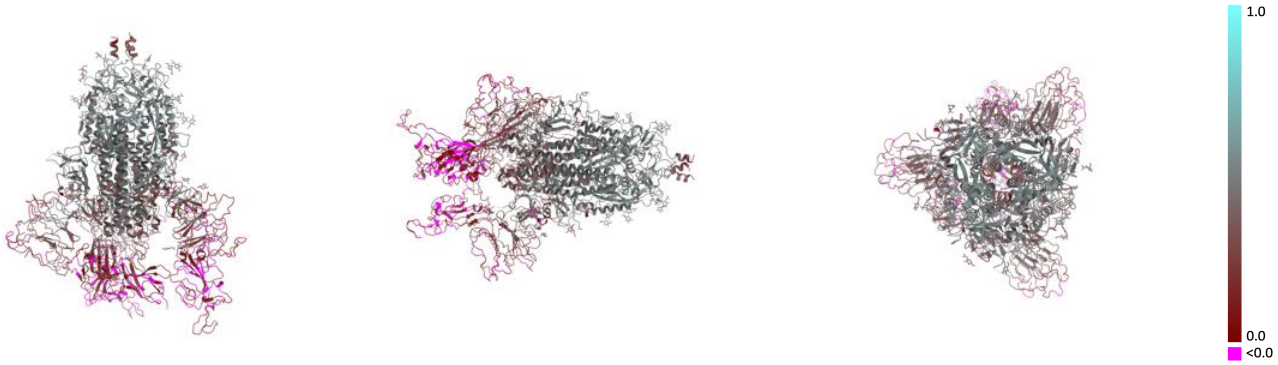
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

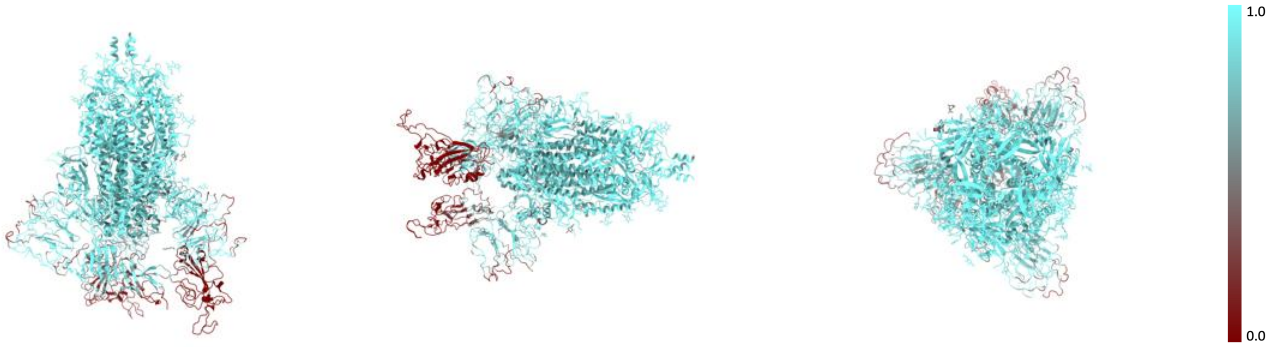
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

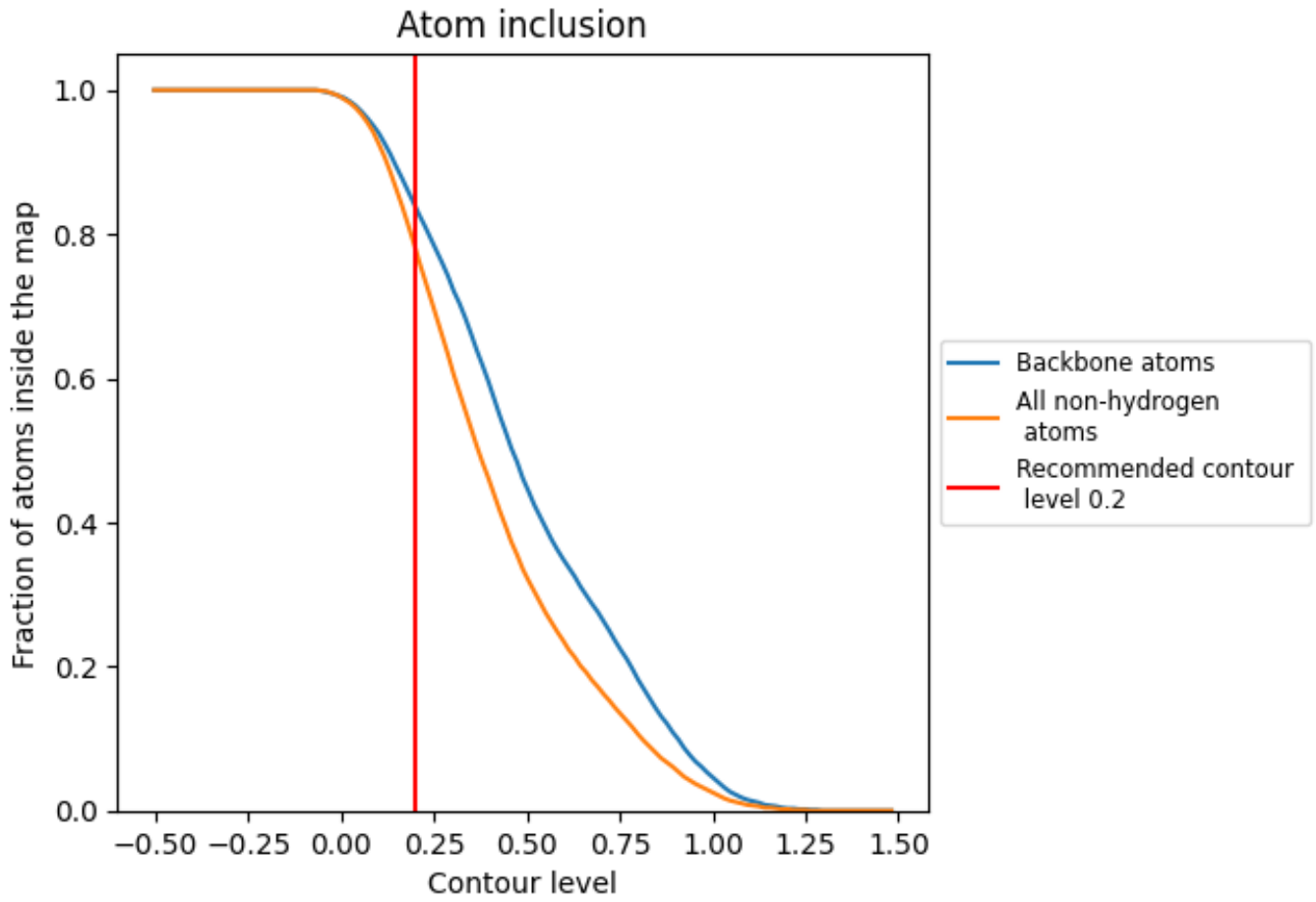
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.3340
A	0.7170	0.3220
B	0.7690	0.3500
C	0.8770	0.3560
I	0.4960	0.1060
J	0.5710	0.1040
K	0.9290	0.4650
L	0.9290	0.4290
M	0.8930	0.4130
N	0.9640	0.4450
R	0.8930	0.4320
S	0.8570	0.4030
T	0.9640	0.3370
U	0.9290	0.4480
X	0.9290	0.4720
Y	0.9290	0.4020
Z	0.9640	0.3760
a	0.9640	0.3620

